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Variable order panel clustering (extended version)

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Abstract

We present a new version of the panel clustering method for a sparse representation of boundary integral equations. Instead of applying the algorithm separately for each matrix row (as in the classical version of the algorithm) we employ more general block partitionings. Furthermore, a variable order of approximation is used depending on the size of blocks.

We apply this algorithm to a second kind Fredholm integral equation and show that the complexity of the method only depends linearly on the number, say n, of unknowns. The complexity of the classical matrix oriented approach is $O(n^2)$ while, for the classical panel clustering algorithm, it is $O(n \log^7 n)$.

1 Introduction

Elliptic boundary value problems with constant coefficients can be transformed into integral equations on the boundary of the domain via the method of integral equations. From the numerical point of view, this approach is interesting especially for problems on unbounded domains where the direct discretization with finite element or finite differences is not straightforward.

Boundary integral equations are discretised in many engineering applications via the boundary element method by lifting conventional finite element spaces onto the surface of the domain. Due to the non-localness of the integral operators the arising system of equations is fully populated. Hence, the work for the classical matrix-oriented approach grows quadratically in the number (n) of unknowns.

In [6], [7], and [11], the panel clustering algorithm was introduced for collocation methods. By using polynomial approximations of the kernel function of the integral operator it was possible to split the dependence of the integration variable from the source points. The algorithm was applied for each matrix row separately. In [7], it was shown that the complexity of the algorithm is proportionally to $O(n \log^{\kappa} n)$ with moderate κ . In [15], [8], [13], [5], the panel clustering algorithm was introduced for the Galerkin discretization of boundary integral equations. The key role plays a symmetric factorization of the kernel function with respect to both variables. Again, the algorithm is applied to each matrix row separately.

In [12], [2], the fast multipole method was introduced for the efficient evaluation of sums in multiple particle systems. Here, the algorithm was applied not pointwise but appropriate block partitionings are employed. The complexity of the algorithm is again proportionally to $O(n \log^k n)$. In [10], a block version of the panel clustering algorithm was introduced. The complexity is still $O(n \log^k n)$ while the constants in the complexity estimates are smaller than for the classical approach.

In our paper, we introduce a variable order approximation on the clusters resulting in an algorithm with complexity O(n). As a model problem we consider a Galerkin discretization of a second kind Fredholm integral equation. The fact that boundary integral equations can be realized (with full stability and consistency) in O(n) operations whilst the classical matrix oriented approach has complexity $O(n^2)$ seems to be of interest. Generalizations of our approach to more general integral equations are the topic of future research.

Another way of a sparse approximation of boundary integral operators are wavelet discretizations. In the past decade they were intensively developed for boundary integral equations. There are versions for second kind integral equations by [18], [17] (complexity $O(n \log^{\kappa} n)$). The approach presented in [16] reduces the complexity to O(n). However, the efficiency of wavelet methods depends on the number of (smooth) charts being employed for the representation of the surface. If the surface is rough and complicated the efficiency breaks down while the panel clustering method works especially well for complicated surfaces.

An algebraic approach to the data-sparse realization of non-local operators are \mathcal{H} -matrices (see [3], [4]). Matrix blocks are approximated by low rank matrices. The choice of the approximation system can be based on a singular value decomposition and is suited to approximate inverses of sparse matrices efficiently.

In this paper, various notations and conventions will be used. In order to improve readability, we have collected below the most relevant ones along with a link to their first appearance.

Notations:

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kernel function (see (2)),
k_{\mathbf{c}}^{(m)}
                              panel clustering approximation (see Assumption 20) and (27),
\Phi_c^{(\nu)}, \Psi_c^{(\mu)}
                             expansion system (see Definition 32),
                              coefficients appearing in the shift of the expansion system
\gamma_{\nu,\tilde{\nu},\tilde{c}}
                              (see (45)),
\begin{array}{l} \check{k}_{\mathbf{c}}^{(m)} \\ \check{\Phi}_{c}^{(\nu)}, \check{\Psi}_{c}^{(\mu)} \end{array}
                              auxiliary Taylor approximation of k (see (22)),
                              auxiliary (Taylor) expansion system (see (23)),
N_c^{(\nu)}, \check{N}_c^{(\nu)}
                             auxiliary expansion functions (see (71), (72)),
A_c^{(\nu)}[u], B_c^{(\nu)}[u], B_{\tau}
                              partial sums related to the panel clustering representation
                              (\text{see }(29), (50), (51)),
B_{\omega}, M_{\omega}, \rho_{\omega}
                              Cebyšev ball, centre, radius (cluster ball, centre, radius)
                              (see Definition 5),
                             approximate cluster radius (see (38)),
\tilde{
ho}_c
                             maximal side length of circumscribing box b_c (see (38)),
\rho, h
                              minimal element radius, step size (see (31), (32)),
\overline{P}^{(2)}, N, F
                              covering of \Gamma \times \Gamma, nearfield, farfield (see Definition 14 and (8)),
                              Cluster/block level, maximal depth of the tree (see Definition
LEVEL. L
                              10 and (35)),
m(c), m(c), m(\ell)
                             Distribution of approximation order (see (16), Remark 41,
                             Definition 60),
\iota_m^{I,II},\ \iota_m,\ \iota_c,\ \iota_{\mathbf{c}}
                             Index sets (see Assumption 20, Definition 32, Notation 34),
REF, INVREF
                              Mapping / pullback to reference tree (see (36)),
\mathcal{L}_{k}^{(i)}\left(\omega\right)
                             Layers around \omega (see Definition 26).
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For a set M, we write $\bigcup M$ short for $\bigcup_{m \in M} M$. The area of a surface piece $\gamma \subset \Gamma$ is denoted by $|\gamma|$.

Throughout the paper, we use the convention that, for a finite element function u, its coefficient vector in the basis representation is denoted by \mathbf{u} .

Similarly, a block of clusters is denoted by \mathbf{c} (bold) while its components are c_1 , c_2 , indicating the correspondence $\mathbf{c} = (c_1, c_2)$.

Two approximation systems will appear for the approximation of the kernel function. One corresponds to the variable order panel clustering approximation and one has auxiliary character. All quantities being related to the auxiliary function system are denoted with a superscript $\check{\cdot}$, as, e.g., \check{k} , $\check{\Phi}$, etc., while the true expansion system is denoted without a superscript.

2 Setting

Let $\Gamma \subset \mathbb{R}^3$ denote an orientable, sufficiently smooth manifold ($\Gamma \in C^2$ is sufficient). On Γ , we consider the integral equation with the classical double layer potential in the weak form: For given $f \in L^2(\Gamma)$, find $u \in L^2(\Gamma)$ so that

$$2\pi (v, u)_{0,\Gamma} + (v, Ku)_{0,\Gamma} = (v, f)_{0,\Gamma}, \qquad \forall v \in L^{2}(\Gamma)$$
 (1)

holds with

$$K[u](x) = \int_{\Gamma} k(x, y) u(y) ds_{y},$$

$$k(x, y) = \frac{\partial}{\partial n(y)} \frac{1}{\|x - y\|}.$$
(2)

Here, $L^2(\Gamma)$ denotes the set of all measurable functions on Γ which are square integrable and $(\cdot, \cdot)_{0,\Gamma}$ the L^2 -scalar product on Γ . The vector field n(y) denotes the oriented normal vector field at a surface point $y \in \Gamma$.

The Galerkin discretization of (1) is given by replacing the infinite dimensional space $L^2(\Gamma)$ by a finite dimensional subspace \mathcal{V} . The Galerkin solution u_G is the solution of

$$2\pi (v, u_G)_{0,\Gamma} + (v, Ku_G)_{0,\Gamma} = (v, f)_{0,\Gamma}, \qquad \forall v \in \mathcal{V}.$$
(3)

Our aim is to use finite element spaces lifted to the manifold Γ as the subspace \mathcal{V} . Finite element spaces are defined on finite element grids. We introduce the two-dimensional master triangle Q having the vertices $(0,0)^{\mathsf{T}}$, $(1,0)^{\mathsf{T}}$, $(1,1)^{\mathsf{T}}$.

Definition 1 A finite element grid of Γ is a set $\mathcal{G} = \{\tau_1, \tau_2, \dots, \tau_n\}$ consisting of disjoint, open surface pieces $\tau_i \subset \Gamma$ satisfying

- $\overline{\Gamma} = \overline{\bigcup \mathcal{G}}$,
- for all $\tau \in \mathcal{G}$, there exists a C^k -diffeomorphism $\chi_{\tau}: Q \to \tau$ (k sufficiently large) which can be extended to a C^k -diffeomorphism $\chi_{\tau}^{\star}: Q^{\star} \to \tau^{\star}$ for some open neighbourhoods $\tau^{\star} \supset \overline{\tau}$ and $Q^{\star} \supset \overline{Q}$.

Notation 2 The elements of a finite element grid are called "geometric finite elements". In the context of boundary element methods they are alternatively called "panels".

In this paper, we restrict to piecewise constant approximations on triangulations.

Definition 3 The space $S^{-1,0}$ is given by

$$S^{-1,0} = \left\{ v \in L^2 \left(\Gamma \right) : \forall \tau \in \mathcal{G} : v \mid_{\tau} = const \right\}.$$

A local basis of $S^{-1,0}$ is formed by the characteristic functions on the triangles:

$$b_{\tau} : \Gamma \to \mathbb{R},$$

$$\forall \tau \in \mathcal{G} : b_{\tau}(x) = \begin{cases} 1 & x \in \tau, \\ 0 & \text{otherwise.} \end{cases}$$

By using the basis representation

$$u_G(x) = \sum_{\tau \in \mathcal{G}} \mathbf{u}_G(\tau) b_{\tau}(x), \qquad (4)$$

the Galerkin discretization can be transformed into a system of linear equations:

$$(\mathbf{M} + \mathbf{K}) \mathbf{u}_G = \mathbf{g}$$

where $\mathbf{M}, \mathbf{K} \in \mathbb{R}^{\mathcal{G} \times \mathcal{G}}$ and $\mathbf{u}_G, \mathbf{g} \in \mathbb{R}^{\mathcal{G}}$ are given, for all $\tau, t \in \mathcal{G}$, by

$$\mathbf{M}_{\tau,t} = 2\pi \left(b_{\tau}, b_{t}\right)_{0,\Gamma}, \qquad \mathbf{u}_{G} = \left(u_{G} \mid_{\tau}\right)_{\tau \in \mathcal{G}}, \\ \mathbf{K}_{\tau,t} = \left(b_{\tau}, K \left[b_{t}\right]\right)_{0,\Gamma}, \qquad \mathbf{g} = \left(\left(b_{\tau}, f\right)_{0,\Gamma}\right)_{\tau \in \mathcal{G}}.$$

The matrix **M** is diagonal while **K** is a fully populated $n \times n$ -matrix. Hence, the classical matrix oriented approach costs (at least) $O(n^2)$ operations.

The idea of the panel clustering method is to use an alternative representation of the discrete integral operator which can be written in the form

$$\mathbf{K} \approx \mathbf{N} + \mathbf{B}^{\mathsf{T}} \mathbf{F} \mathbf{C},$$
 (5)

where the matrix \mathbf{N} is sparse containing only O(n) non-zero entries. Furthermore, $\mathbf{B}, \mathbf{C} \in \mathbb{C}^{m \times n}$ with $m \ll n$ and $\mathbf{F} \in \mathbb{C}^{m \times m}$. Note that, by using this representation, the matrix elements of \mathbf{K} are not known, i.e., direct solvers cannot be applied to this system. However, for large n, iterative solvers are much more efficient than direct solvers and should be used instead. For iterative solvers, the matrix elements of \mathbf{K} are not required. Matrix-vector multiplications appear as elementary operations which can be performed efficiently by using the splitting (5). The rest of the paper is concerned with the definition and analysis of an approximate factorization of the integral operator in (3).

First, we have to introduce some geometric notations.

Definition 4 A cluster is the union of one or more panels.

The geometric size of a cluster can be described via the Čebyšev radius of the cluster.

Definition 5 For a subset $\omega \subset \mathbb{R}^d$, the Čebyšev ball B_ω is the ball with minimal radius containing ω . The Čebyšev centre M_ω is the midpoint of this ball and the Čebyšev radius ρ_ω its radius.

Notation 6 For a cluster c, the Čebyšev ball, Čebyšev centre, and Čebyšev radius are alternatively denoted by cluster ball, cluster centre, and cluster radius.

For the efficiency of the algorithm, it is important to organize the clusters in a hierarchical tree. In this light, a set (set of sons) has to be associated with each cluster.

Definition 7 A set of sons $\sigma(c)$ associated with a cluster c

- 1. is either the empty set,
- 2. or is the union of one or more disjoint clusters satisfying

$$\overline{c} = \overline{\bigcup \sigma\left(c\right)}.$$

3. If $\sigma(c) = \emptyset$ then $c \in \mathcal{G}$.

A cluster c with $\sigma(c) = \emptyset$ is called a *leaf*.

Definition 8 A cluster tree T corresponding to a grid G consists of clusters with associated sets of sons satisfying:

- 1. $\Gamma \in T$.
- 2. Any $c \in T$ with associated set of sons $\sigma(c)$ satisfies either
 - (a) $\sigma(c) = \emptyset$,
 - (b) $\overline{c} = \overline{\bigcup \sigma(c)}$.

Remark 9 We do not require that $\sharp \sigma(c) \neq 1$. For the later constructions, it will be convenient to allow $\sharp \sigma(c) = 1$ implying $\tilde{c} = c$ for $\tilde{c} \in \sigma(c)$.

In the next step, we will associate to each cluster a level indicating the depth in the cluster tree. Since the largest cluster, i.e., the surface Γ , is subdivided recursively into smaller clusters, it is natural to use the depth of a cluster τ as an indication of the geometric size as well.

Definition 10 The function LEVEL: $T \to \mathbb{N}_0$ is the recursive function

$$LEVEL(\Gamma) = 0,$$

$$LEVEL(\tilde{c}) = LEVEL(c) + 1, \quad \forall \tilde{c} \in \sigma(c), \quad \forall c \in T \setminus \mathcal{G}.$$

The depth of the cluster tree is

$$L = \max \{ \text{LEVEL}(c) : c \in T \}$$

while the **minimal depth** is given by

$$L_{\min} := \min \left\{ \text{LEVEL} \left(\tau \right) : \tau \in \mathcal{G} \right\}. \tag{6}$$

For $0 \le \ell \le L$, the **tree level** $T(\ell)$ contains all clusters $c \in T$ with LEVEL $(c) = \ell$.

The term $(v, Ku)_{0,\Gamma}$ in (3) contains an integral over $\Gamma \times \Gamma$:

$$(v, Ku)_{0,\Gamma} = \int_{\Gamma \times \Gamma} v(x) u(y) k(x, y) ds_y ds_x.$$

In the next step, the product $\Gamma \times \Gamma$ is partitioned into pairs of clusters defining a block partitioning of $\Gamma \times \Gamma$. A pair $\mathbf{c} = (c_1, c_2) \in T \times T$ is called a *block*.

Definition 11 Let $\eta \in (0,1)$. A block $\mathbf{c} \in T \times T$ is η -admissible if

$$\max\left\{\rho_{c_1}, \rho_{c_2}\right\} \le \eta \operatorname{dist}\left(c_1, c_2\right) \tag{7}$$

holds with ρ_{c_1}, ρ_{c_2} as in Definition 5.

If there is no ambiguity we write "admissible" short for " η -admissible".

Definition 12 Let $\mathbf{c} = (c_1, c_2) \in T \times T$. The set of sons of \mathbf{c} is given by

- $\sigma(\mathbf{c}) = \sigma(c_1) \times \sigma(c_2)$ provided $\sigma(c_1) \neq \emptyset$ and $\sigma(c_2) \neq \emptyset$,
- $\sigma(\mathbf{c}) = \sigma(c_1) \times \{c_2\}$ provided $\sigma(c_1) \neq \emptyset$ and $\sigma(c_2) = \emptyset$,
- $\sigma(\mathbf{c}) = \{c_1\} \times \sigma(c_2) \text{ provided } \sigma(c_1) = \emptyset \text{ and } \sigma(c_2) \neq \emptyset,$
- $\sigma(\mathbf{c}) = \emptyset$ provided $\sigma(c_1) = \sigma(c_2) = \emptyset$.

A block $\mathbf{c} \in T \times T$ is called a leaf if $\sigma(\mathbf{c}) = \emptyset$. The tree T induces a block cluster tree $T^{(2)}$ of $\Gamma \times \Gamma$.

Definition 13 $T^{(2)}$ is a block cluster tree if

- $(\Gamma, \Gamma) \in T^{(2)}$,
- every $\mathbf{c} \in T^{(2)}$ satisfies one of the alternatives:
 - **c** is a leaf,
 - $\overline{\mathbf{c}} = \overline{\bigcup \sigma(\mathbf{c})}.$

Note that the block cluster tree $T^{(2)}$ is fully determined by the cluster tree T.

Definition 14 A subset $P^{(2)} \subset T^{(2)}$ is a block partitioning of $\Gamma \times \Gamma$ if the elements of $P^{(2)}$ are disjoint and

$$\overline{\Gamma \times \Gamma} = \overline{\bigcup P^{(2)}}.$$

It is an η -admissible block partitioning if every $\mathbf{c} \in P^{(2)}$ satisfies one of the alternatives

- c is a leaf,
- **c** is η -admissible.

It is a minimal, η -admissible block partitioning if there is no η -admissible block partitioning with less elements.

Algorithm 15 The minimal, η -admissible block partitioning of $\Gamma \times \Gamma$ is obtained as the result of the procedure $divide((\Gamma, \Gamma), \emptyset)$ defined by (see [7])

```
procedure divide(c, P);
begin
if (c is a leaf) then P := P \cup \{c\}
else if (c is admissible) then P := P \cup \{c\}
else for all \widetilde{\mathbf{c}} \in \sigma(\mathbf{c}) do divide(\widetilde{\mathbf{c}}, P);
end;
```

The partitioning P_{\min} contains non-admissible leaves and admissible blocks. These subsets are denoted by N (nearfield) and F (farfield):

$$N := \{ \mathbf{c} \in P_{\min} : \mathbf{c} \text{ is non-admissible} \},$$

$$F := P_{\min} \backslash N.$$
(8)

On blocks $\mathbf{c} \in F$, the kernel function will be replaced by an approximation of a certain order. The idea is that, on blocks consisting of clusters of similar size, the approximation order is the same and, in addition, the approximation order is smaller on smaller blocks.

Definition 16 Let L_{\min} be as in (6). The order distribution function $m: F \to \mathbb{N}_0$ depends on two constants $a, b \in \mathbb{N}_0$ and is given by

$$m(\mathbf{c}) := a \left(L_{\min} - \ell_{\min}(\mathbf{c}) \right)_{\perp} + b \tag{9}$$

with

$$\ell_{\min}\left(\mathbf{c}\right) = \min\left\{\text{LEVEL}\left(c_{1}\right), \text{LEVEL}\left(c_{2}\right)\right\}$$

and

$$(\cdot)_{+} = \max\left\{0, \cdot\right\}.$$

The order distribution is extended to a function $m: F \cup T \to \mathbb{N}_0$ by

$$m(c) = \max \{ m(\mathbf{c}) : \mathbf{c} \in F \land c \in \{c_1, c_2\} \}, \qquad c \in T.$$

$$(10)$$

Remark 17 One could generalise the function m by allowing $a, b \in \mathbb{R}_{>0}$ and defining

$$m\left(\mathbf{c}\right) := \left[a\left(L_{\min} - \ell_{\min}\left(\mathbf{c}\right)\right)_{+} + b\right],$$

where [x] denotes the smallest integer larger than or equal to x.

Remark 18 Definition 16 implies that the approximation order on a block (c_1, c_2) is determined by the "larger cluster" $c = \operatorname{argmin} \{ \operatorname{LEVEL}(c_1), \operatorname{LEVEL}(c_2) \}$. The approximation order is high on large clusters, e.g., $m(\Gamma, \Gamma) = aL_{\min} + b$ and small for small clusters as, e.g., 1

$$m\left(c_{1},c_{2}\right)=b$$

for all c_1, c_2 satisfying LEVEL (c_1) , LEVEL $(c_2) \geq L_{\min}$.

Remark 19 In Subsection 3.1, a construction for the sets T, $P^{(2)}$ is presented which always guarantees that $(c_1, c_2) \in P^{(2)}$ implies that c_1 and c_2 belong to the same $T(\ell)$ for some ℓ . In this case, the order distribution m only depends on the level ℓ .

3 The variable order panel clustering algorithm

In this section, we will define the panel clustering algorithm. In the previous section, we have defined a partitioning of $\Gamma \times \Gamma$ into a minimal, η -admissible block partitioning $P_{\min} = N \cup F$. On the portion $\bigcup N \subset \Gamma \times \Gamma$, the standard, matrix oriented approach is used while, on $\bigcup F$, the kernel function is approximated by suitable expansions. Let the kernel function k be as in (2).

Assumption 20 There exist positive constants C_1 , C_3 , C_4 , $C_5 \in \mathbb{R}_{>0}$, integers λ_1 , $\lambda_I, \ \lambda_{II}, \ d_I, \ d_{II} \in \mathbb{N}_0 \ and \ C_2, \overline{\eta} \in (0,1) \ having the following properties. For all$ $\eta \in (0, \overline{\eta})$ and all η -admissible block partitionings $P^{(2)}$ of $\Gamma \times \Gamma$, for all $\mathbf{c} \in F$, there is a family of approximations $k_{\mathbf{c}}^{(m)}$, $m \in \mathbb{N}_0$, of the kernel function k satisfying

$$|k(x,y) - k_{\mathbf{c}}^{(m)}(x,y)| \le C_1 C_2^m \operatorname{dist}^{-1}(c_1, c_2), \quad \forall (x,y) \in \mathbf{c}.$$
 (11)

having the form

$$k_{\mathbf{c}}^{(m)}(x,y) = \sum_{(\nu,\mu)\in\mathbf{I}_{m}} \kappa_{\nu,\mu}^{(m)}(\mathbf{c}) \,\Phi_{c_{1}}^{(\nu)}(x) \,\Psi_{c_{2}}^{(\mu)}(y) \tag{12}$$

with index sets $\mathbf{I}_m \subset \mathbb{N}_0^{d_I} \times \mathbb{N}_0^{d_{II}}$, $m \in \mathbb{N}_0$, satisfying

$$\sharp \mathbf{I}_m \leq C_3 (m+1)^{\lambda_1}, \qquad (13)$$

$$\iota_m^I := \left\{ \nu \mid \exists \mu \in \mathbb{N}_0^{d_I} : (\nu, \mu) \in \mathbf{I}_m \right\}, \tag{14}$$

$$\iota_m^{II} := \left\{ \mu \mid \exists \nu \in \mathbb{N}_0^{d_{II}} : (\nu, \mu) \in \mathbf{I}_m \right\}, \tag{15}$$

$$\sharp \iota_m^s \leq C_4 (m+1)^{\lambda_s}, \qquad s \in \{I, II\},$$
(16)

$$|\nu| \leq C_5 (m+1), \quad \forall \nu \in \iota_m^s, \quad s \in \{I, II\},$$
 (17)

$$|\nu| \leq C_5 (m+1), \quad \forall \nu \in \iota_m^s, \quad s \in \{I, II\},$$

$$\iota_m^I \subset \iota_M^{II}, \quad \iota_m^{II} \subset \iota_M^{II}, \quad \forall 0 \leq m \leq M.$$

$$(18)$$

¹For a block $\mathbf{c} = (c_1, c_2)$, the notation $m(c_1, c_2)$ is short for $m((c_1, c_2))$.

The approximation of the kernel function is based on a modification of Taylor expansions. In this light, we begin with analysing the (true) Taylor approximation of the kernel function $k_{\mathbf{c}}^{(m)}$ and, then, explain the modification. We begin with introducing some notations.

For $\mathbf{c} \in F$, the difference domain $d(\mathbf{c})$ is given by

$$d(\mathbf{c}) = c_1 - c_2 = \left\{ z \in \mathbb{R}^3 \mid \exists (x, y) \in \mathbf{c} : z = x - y \right\}.$$
 (19)

Put $z_{\mathbf{c}} = M_{c_1} - M_{c_2}$ (cf. Definition 5). One easily checks that, since \mathbf{c} is admissible, $z_{\mathbf{c}} \neq 0$. The kernel function in relative coordinates defines the function $k_{rel} : c_1 \times d(\mathbf{c}) \to \mathbb{R}$

$$k_{rel}(y, z) = \langle n(y), z \rangle k_3(z)$$

with

$$k_3(z) := \frac{1}{\|z\|^3}. (20)$$

Taylor expansion of k_3 about z_c yields (writing n short for n(y)):

$$k_{rel,\mathbf{c}}^{(m)}(y,z) = \langle n, z \rangle \sum_{|\nu| < m} \frac{(z - z_{\mathbf{c}})^{\nu}}{\nu!} k_3^{(\nu)}(z_{\mathbf{c}}), \qquad (21)$$

where we employed the usual multi-index notation for $\nu \in \mathbb{N}_0^3$. Re-substituting z = x - y, factorizing $(x - y - z_c)^{\nu}$ with respect to $x - M_{c_1}$ and $y - M_{c_2}$, and rearranging the terms results in²

$$\check{k}_{\mathbf{c}}^{(m)}(x,y) := k_{rel,\mathbf{c}}^{(m)}(y,x-y) = \sum_{i=1}^{3} \sum_{|\nu|+|\mu| \le m} (x - M_{c_1})^{\nu} n_i (y - M_{c_2})^{\mu} \kappa_{\nu,\mu,i}^{(m)}(\mathbf{c}) \quad (22)$$

with

$$\kappa_{\nu,\mu,i}^{(m)}(\mathbf{c}) = \frac{(-1)^{|\mu|}}{\mu!\nu!} \begin{cases} (\nu_i + \mu_i) k_3^{(\nu+\mu-e_i)}(z_{\mathbf{c}}) + (z_{\mathbf{c}})_i k_3^{(\nu+\mu)}(z_{\mathbf{c}}) & |\nu| + |\mu| < m, \\ (\nu_i + \mu_i) k_3^{(\nu+\mu-e_i)}(z_{\mathbf{c}}) & |\nu| + |\mu| = m. \end{cases}$$

Here, $\{e_i\}_{i=1}^3$ denotes the set of canonical unit vectors in \mathbb{R}^3 . Introducing the seven-dimensional index set:

$$\widetilde{\mathbf{I}}_m = \{(\nu, \mu, i) \in \mathbb{N}_0^3 \times \mathbb{N}_0^3 \times \{1, 2, 3\} : |\nu| + |\mu| \le m \}.$$

and the function system

$$\check{\Phi}^{(\nu)}(x) = (x - M_{c_1})^{\nu}, \qquad \check{\Psi}^{(\mu,i)}(y) = (y - M_{c_2})^{\mu} n_i(y) \tag{23}$$

For the variable order panel clustering algorithm, the functions $(\cdot - M_c)^{\nu}$ will be replaced by suitable approximations. This is the reason why we denote the function in (22) by $\check{k}_{\mathbf{c}}^{(m)}$ instead of $k_{\mathbf{c}}^{(m)}$.

results in an expansion of the form (12). In order to reduce the number of indices the three-dimensional coefficients and functions \overrightarrow{k} and $\overrightarrow{\Psi}_c$ are introduced by

$$\overrightarrow{\kappa}_{\nu,\mu}^{(m)}\left(\mathbf{c}\right) = \left\{\kappa_{\nu,\mu,i}^{(m)}\left(\mathbf{c}\right)\right\}_{i=1}^{3}, \qquad \overrightarrow{\check{\Psi}}^{(\mu)} = \left\{\check{\Psi}^{(\mu,i)}\left(y\right)\right\}_{i=1}^{3}.$$

The expansion (22) can be rewritten as

$$\check{k}_{\mathbf{c}}^{(m)} = \sum_{(\nu,\mu) \in \mathbf{I}_m} \check{\Phi}_c^{(\nu)} \overrightarrow{\check{\Psi}}_c^{(\mu)} \overrightarrow{\kappa}_{\nu,\mu}^{(m)} \left(\mathbf{c} \right)$$

with the six-dimensional index set

$$\mathbf{I}_m = \{ (\nu, \mu) \in \mathbb{N}_0^3 \times \mathbb{N}_0^3 : |\nu| + |\mu| \le m \}$$

and the convention

$$\overrightarrow{\underline{\Psi}}_{c}^{(\mu)} \overrightarrow{\kappa}_{\nu,\mu}^{(m)} (\mathbf{c}) = \sum_{i=1}^{3} \underline{\Psi}_{c}^{(\mu,i)} \kappa_{\nu,\mu,i}^{(m)} (\mathbf{c}).$$

In [7, Appendix A], it was proved that there exists constants \widetilde{C}_1 , \widetilde{C}_2 , and $\widetilde{\eta}_0$ so that

$$\left| k\left(x,y \right) - \check{k}_{\mathbf{c}}^{(m)}\left(x,y \right) \right| \leq \widetilde{C}_{1} \left(\widetilde{C}_{2} \widetilde{\eta} \right)^{m} \left| k\left(x,y \right) \right| \tag{24}$$

holds for all $(x, y) \in \mathbf{c}$ satisfying $||x - y - z_{\mathbf{c}}|| \le \tilde{\eta} ||z_{\mathbf{c}}||$ and all $\tilde{\eta} \in (0, \tilde{\eta_0})$.

Lemma 21 Let $P^{(2)}$ denote an η -admissible block partitioning of $\Gamma \times \Gamma$ with $\eta \in (0, \overline{\eta})$ and $\overline{\eta} := \min\left\{\frac{1}{4}, \frac{1}{5\widetilde{C_2}}\right\}$. Then, Assumption 20 is satisfied.

Proof. Since the block partitioning was assumed to be η -admissible we conclude:

$$||x - y - z_{\mathbf{c}}|| \le ||x - M_{c_1}|| + ||y - M_{c_2}|| \le \rho_{c_1} + \rho_{c_2} \le 2\eta \operatorname{dist}(c_1, c_2).$$

The distance can be estimated by:

$$\operatorname{dist}(c_1, c_2) \leq \|M_{c_1} - M_{c_2}\| + \rho_{c_2} + \rho_{c_1} \leq \|M_{c_1} - M_{c_2}\| + 2\eta \operatorname{dist}(c_1, c_2).$$

Using $\eta < \frac{1}{4}$ we get

$$dist(c_1, c_2) \le 2 \|M_{c_1} - M_{c_2}\|$$

and, finally,

$$||x - y - z_{\mathbf{c}}|| \le 4\eta ||z_{\mathbf{c}}||.$$

By choosing $\bar{\eta} = \widetilde{\eta_0}/4$ in Assumption 20 with $\widetilde{\eta_0}$ as in (24) results in $4\eta =: \tilde{\eta} \in (0, \widetilde{\eta_0})$ in (24). Hence, (11) holds with $C_2 = 4\widetilde{C_2}\eta < 4/5$. Let C_{Γ} denote the smallest constant so that, for all $\mathbf{c} \in P^{(2)}$ and all $(x, y) \in \mathbf{c}$:

$$|\langle n(y), x - y \rangle| \le C_{\Gamma} ||x - y||^2$$
.

Then,

$$|k(x,y)| = \frac{\langle n(y), x - y \rangle}{\|x - y\|^3} \le C_{\Gamma} \frac{1}{\|x - y\|} \le C_{\Gamma} \operatorname{dist}^{-1}(c_1, c_2), \quad \forall (x, y) \in \mathbf{c}$$

and Assumption 20 is satisfied for $k_{\mathbf{c}}^m = \check{k}_{\mathbf{c}}^{(m)}$ with $C_1 = \widetilde{C}_1 C_{\Gamma}$. Some combinatorial manipulations yield

$$\sharp \tilde{\mathbf{I}}_m \le 3 (m+1)^6$$
, i.e., $C_3 = 3$, $\lambda_1 = 6$.

Obviously:

$$\iota_m^I = \left\{ \nu \in \mathbb{N}_0^3 : |\nu| \le m \right\} \tag{25}$$

$$\tilde{\iota}_{m}^{II} = \left\{ \nu \in \mathbb{N}_{0}^{3} : |\nu| \le m \right\} \times \{1, 2, 3\}.$$
 (26)

Again, some combinatorial manipulations lead to

$$C_4 = 3,$$
 $\lambda_1^I = \lambda_2^{II} = 3,$ $d_I = 3,$ $d_{II} = 4.$

Finally, $C_5 = 2$ is trivial.

In [15], [8], it was proved that all kernel functions corresponding to elliptic boundary value problems admit an approximation satisfying Assumption 20.

Remark 22 For the variable order panel clustering algorithm, the Taylor-based expansion derived in the previous example will be modified by replacing the expansion functions (23) by approximations having more hierarchical structure with respect to the order m.

Remark 23 The panel clustering method is by no means linked to Taylor based expansions. Other expansions as, e.g., expansions in spherical harmonics could be preferable for special applications.

The panel clustering approximation of $(v, Ku)_{0,\Gamma}$ is given by

$$(v, Ku)_{0,\Gamma} \approx \sum_{\mathbf{c} \in N} \int_{\mathbf{c}} v(x) u(y) k(x, y) ds_{x} ds_{y}$$

$$+ \sum_{\mathbf{c} \in F} \sum_{(\nu, \mu) \in \mathbf{I}_{m(\mathbf{c})}} \overrightarrow{\kappa}_{\nu, \mu}^{(m)}(\mathbf{c}) \int_{c_{1}} \Phi_{c_{1}}^{(\nu)}(x) v(x) ds_{x} \int_{c_{2}} \overrightarrow{\Psi}_{c_{2}}^{(\mu)}(y) u(y) ds_{y}.$$

$$(27)$$

The function $m(\mathbf{c})$ determines the order of approximation on blocks $\mathbf{c} \in F(\ell)$. It was defined in Definition 16 while the constants $a, b \in \mathbb{N}_0$ will be fixed in Definition 60. Assumption 20 implies

$$\mathbf{I}_{m(\mathbf{c})} \subset \iota_{m(\mathbf{c})}^{I} \times \iota_{m(\mathbf{c})}^{II}.$$

Let $\mathbf{c} = (c_1, c_2) \in F$. Then, $m(c_i) \geq m(\mathbf{c})$ for i = 1, 2 (cf. (10)), resulting in

$$\mathbf{I}_{m(\mathbf{c})} \subset \iota_{m(c_1)}^I \times \iota_{m(c_2)}^{II}. \tag{28}$$

Property (28) will allow to decompose the computations related to the index set $\mathbf{I}_{m(\mathbf{c})}$ into separate computations on the index sets $\iota^{I}_{m(c_1)}$, $\iota^{II}_{m(c_2)}$.

For the evaluation of a matrix-vector multiplication, expression (27) has to be evaluated for all basis functions $v = b_{\tau}$, $\tau \in \mathcal{G}$.

The variable order panel clustering algorithm

The variable order panel clustering algorithm depends on various parameters:

- η : The constant appearing in the definition of η -admissibility.
- The choice of the constants a, b in the definition of $m = m(\mathbf{c})$ (as in (9)) in (11). The precise choice of a and b is given in Definition 60.

Setup phase:

- 1. For a given mesh \mathcal{G} , build up the cluster tree T and compute all cluster radii and cluster centres.
- 2. Compute P_{\min} by using the procedure **divide** of Algorithm 15.
- 3. For all farfield blocks $\mathbf{c} \in F$, $(\nu, \mu) \in \mathbf{I}_{m(\mathbf{c})}$: compute the coefficients $\overrightarrow{\kappa}_{\nu,\mu}^{m(\mathbf{c})}(\mathbf{c})$.
- 4. Compute the nearfield matrix entries:

$$\mathbf{N}_{\tau,t} = \int_{\tau \times t} k(x, y) \, ds_y ds_x, \qquad \forall (\tau, t) \in N.$$

5. For all $\tau \in \mathcal{G}$: compute the basis farfield coefficients:

$$J_{\tau,\nu}^{I} = \int_{\tau} \Phi_{\tau}^{(\nu)}(x) ds_{x}, \qquad \forall \nu \in \iota_{m(\tau)}^{I},$$

$$\overrightarrow{J}_{\tau,\nu}^{II} = \int_{\tau} \overrightarrow{\Psi}_{\tau}^{(\nu)}(x) ds_{x}, \qquad \forall \nu \in \iota_{m(\tau)}^{II}.$$

Evaluation phase:

Let $u \in S^{-1,0}$ and $\mathbf{u} \in \mathbb{R}^{\mathcal{G}}$ so that $u = \sum_{\tau \in \mathcal{G}} \mathbf{u}(\tau) b_{\tau}$ as in (4).

1. Compute the farfield coefficients: For all $c \in T$:

$$\overrightarrow{J}_{c,\mu}^{II}\left[u\right] := \int_{c} \overrightarrow{\Psi}_{c}^{(\mu)}\left(x\right) u\left(x\right) ds_{x}, \qquad \forall \mu \in \iota_{m(c)}^{II}.$$

2. For all $\mathbf{c} = (c_1, c_2) \in P^{(2)}(\ell), \nu \in \iota_{m(\mathbf{c})}^I$:

$$A_{\mathbf{c}}^{(\nu)}\left[u\right] := \sum_{\mu:(\nu,\mu)\in\mathbf{I}_{m(\mathbf{c})}} \overrightarrow{\kappa}_{\nu,\mu}^{m(\mathbf{c})}\left(\mathbf{c}\right) \overrightarrow{J}_{c_{2},\mu}^{II}\left[u\right]. \tag{29}$$

3. Approximate a matrix vector multiplication by

$$\sum_{t \in \mathcal{G}} \mathbf{N}_{\tau, t} \mathbf{u}\left(t\right) + \sum_{\mathbf{c} \in F} \sum_{\nu \in \iota_{m(\mathbf{c})}^{I}} \int_{c_{1}} A_{\mathbf{c}}^{(\nu)}\left[u\right] \Phi_{c_{1}}^{(\nu)}\left(x\right) b_{\tau}\left(x\right) ds_{x}, \qquad \forall \tau \in \mathcal{G}.$$
 (30)

Remark 24 Let $\mathbf{c} = (c_1, c_2) \in F$ and $m_i = m(c_i)$, i = 1, 2. For the realization of the algorithm, it is essential that

$$\mathbf{I}_{m(\mathbf{c})} \subset \iota_{m_1}^I \times \iota_{m_2}^{II}$$

holds. This condition is guaranteed since, in view of (10), we have $m_i \geq m(\mathbf{c})$ and

$$\mathbf{I}_{m(\mathbf{c})} \subset \iota_{m(\mathbf{c})}^{I} \times \iota_{m(\mathbf{c})}^{II} \subset \iota_{m_1}^{I} \times \iota_{m_2}^{II}.$$

In the sequel, we will comment on the realization of the single steps in the algorithm which is essential for both, the practical implementation and the complexity analysis. Some further approximations and relaxations will occur.

3.1 Construction of the cluster tree

Let \mathcal{G} denote the given mesh of Γ . In a first step, one has to compute the centre and radius (cf. Definition 5) of each panel $\tau \in \mathcal{G}$. The smallest radius defines the quantity

$$\underline{\rho} := \min_{\tau \in \mathcal{G}} \rho_{\tau},\tag{31}$$

while the "step size" h of \mathcal{G} is given by

$$h = \max_{\tau \in \mathcal{G}} \operatorname{diam} \tau. \tag{32}$$

We give a construction based on an auxiliary uniform grid with a uniform partitioning. This grid is not needed in the true computations but inherits a simple logical structure to the true grid \mathcal{G} . Let Q denote the smallest cube containing Γ with edges parallel to the coordinate axes. Without loss of generality we may assume that $Q = (0,1)^3$. We introduce a sequence of physically and logically nested grids on Q.

For $\ell \in \mathbb{N}_0$, let $h_{\ell} = 2^{-\ell}$ and $n_{\ell} = 2^{\ell}$. The interval $\pi_{i,\ell}$ is defined, for $1 \leq i \leq n_{\ell}$, by $\pi_{i,\ell} := ((i-1) h_{\ell}, ih_{\ell})$. For $\mu \in (\mathbb{N}_{\leq n_{\ell}})^3$, a cell $q_{\mu,\ell}$ is given by

$$q_{\mu,\ell} = \pi_{\mu_1,\ell} \times \pi_{\mu_2,\ell} \times \pi_{\mu_3,\ell}.$$

Lemma 25 For $\mu \in (\mathbb{N}_{\leq n_{\ell}})^3$ and $\ell \in \mathbb{N}_0$, the radius and centre of $q_{\mu,\ell}$ are given by

$$\rho_{\mu,\ell} : = \rho_{q_{\mu,\ell}} = \sqrt{3} \frac{h_{\ell}}{2},$$

$$M_{\mu,\ell} : = M_{q_{\mu,\ell}} = h_{\ell} \left(\mu - 2^{-1} (1, 1, 1)^{\mathsf{T}} \right).$$
(33)

The reference grid Q_{ℓ} is defined by

$$\mathcal{Q}_{\ell} := \left\{ q_{\mu,\ell} : \mu \in (\mathbb{N}_{\leq n_{\ell}})^3 \right\}. \tag{34}$$

Obviously, each element $q \in \mathcal{Q}_{\ell}$ has exactly eight sons in $\mathcal{Q}_{\ell+1}$ satisfying

$$\overline{q} = \overline{\bigcup \sigma \left(q\right)}.$$

In other words, $\{Q_\ell\}_{\ell\in\mathbb{N}_0}$ is an oct-tree. This tree will be associated to \mathcal{G} . Let L denote the smallest number so that

$$\sqrt{3}\frac{h_L}{2} \le \underline{\rho} \tag{35}$$

holds with $\underline{\rho}$ as in (31). Hence, a cluster tree for the auxiliary grid \mathcal{Q}_L is given by $\mathcal{Q} = \{\mathcal{Q}_\ell\}_{0 < \ell < L}$.

Any element $\tau \in \mathcal{G}$ is associated to that element $q \in \mathcal{Q}_L$ containing the centre of τ . (If there are multiple possibilities, choose one of them). This defines a mapping REF: $\mathcal{G} \to \mathcal{Q}_L$. Since the mapping REF is injective (cf. [4, Remark 5.1]) the pullback is well-defined on Range (REF). In this light we define INVREF: $\mathcal{Q}_L \to \mathcal{G} \cup \{\emptyset\}$ via

INVREF
$$(q) = \begin{cases} \tau & \text{if } q = \text{REF}(\tau) \\ \emptyset & \text{otherwise.} \end{cases}$$
 (36)

The following procedure builds up the cluster tree along with the tree levels. Before we present the formal description of the algorithm we explain the underlying ideas. Our aim is to generate a balanced tree with the additional properties that

- 1. the number of sons of any cluster is different from one,
- 2. the geometric size of a cluster on level $T(\ell)$ is of order $2^{-\ell}$, i.e., there exists $C_7 \geq 1$ so that, for all $c \in T(\ell)$:

$$C_7^{-1} 2^{-\ell} \le \rho_c \le C_7 2^{-\ell}. \tag{37}$$

The cluster ball, centre, and radius are approximated as follows. A box is a rectangular parallelepiped with axes parallel to the coordinate system. For a cluster, it is quite simple to determine the minimal box b(c) containing c. The approximate

cluster ball, centre, and radius are defined as the Čebyšev ball, centre, and radius of b(c) and are denoted by $\tilde{B}(c)$, \tilde{M}_c , and $\tilde{\rho}_c$. By this construction it is guaranteed that

$$c \subset \tilde{B}(c), \qquad s_c/2 \le \rho_c \le \tilde{\rho}_c,$$
 (38)

where s_c denotes the maximal side length of b(c).

The clusters (corresponding to a reference cube $q \in \mathcal{Q}_{\ell}$) are built recursively by collecting the clusters $\bigcup_{\tilde{q} \in \sigma(q)} \{ \text{INVREF}(\tilde{q}) \}$. However, if a cluster contains only one son or the maximal side length s_c is so small that (37) is violated, this cluster is absorbed in the neighbouring cluster. The choice of the neighbouring cluster involves the definition of layers around a set ω .

Definition 26 Let \mathcal{Q}_{ℓ} be as in (34). For $\omega \subset \mathbb{R}^3$, the layers \mathcal{L}_k^i around ω are given by \mathcal{L}_k^0 (ω) := ω and, for $0 \le k \le L$, $i \in \mathbb{N}$, by the recursion:

$$\mathcal{L}_{k}^{1}(\omega) := \bigcup \left\{ q \in \mathcal{Q}_{k} \mid \overline{q} \cap \overline{\omega} \neq \emptyset \right\},$$

$$\mathcal{L}_{k}^{i+1}(\omega) := \mathcal{L}_{k}^{1}\left(\mathcal{L}_{k}^{i}(\omega)\right).$$

If a cluster $c \in T(\ell)$ has only one son or is too small it will be "absorbed" in a "neighbouring" cluster $\tilde{c} \in T(\ell)$ (with reference cluster $\tilde{q} := \text{REF}(\tilde{c})$) satisfying

- 1. $c \subset \mathcal{L}^1_{\ell+1}(\tilde{q})$, i.e., \tilde{c} is "close" to c,
- 2. $s_{\tilde{c}} \geq c_{\min} 2^{-\ell}$, i.e., \tilde{c} is "sufficiently big" (cf. (38)).

The algorithm depends on the parameter $c_{\min} < 1$ controlling the relative smallness of a cluster. The precise choice of c_{\min} is given in Lemma 52.

The recursion starts on the panel level and we put $T(L) = \mathcal{G}$ and $T(L-1) = \emptyset$. On the panel level, we assume that the cluster centres, balls, and radii are computed exactly. Then, the procedure **build_cluster_tree** generates a coarser level from the finer level recursively. As a side result, the mapping REF is extended to all clusters and the pullback INVREF is defined. The procedure is called by

```
\begin{array}{l} \ell := L-1;\\ \mathbf{while}\ T_{\ell+1} \neq \emptyset\ \mathbf{do}\ \mathbf{begin}\\ \mathbf{build\_cluster\_tree}(T_{\ell+1},T_{\ell},\ell)\,;\ell := \ell-1;\\ \mathbf{end}; \end{array}
```

while the procedure **build_cluster_tree** is defined by

```
procedure build_cluster_tree(T_{\ell+1}, T_{\ell}, \ell);
begin
for all q \in \mathcal{Q}_{\ell} do begin c := \emptyset; \sigma(c) := \emptyset; INVREF(q) := \emptyset;
Comment: The sons of the reference cluster q will be collected;
```

```
\begin{array}{ll} \textbf{for all } \tilde{q} \in \sigma\left(q\right) \textbf{ do begin} \\ & \tilde{c} := \text{INVREF}(\tilde{q}) \, ; \qquad c := c \cup \tilde{c}; \\ & \textbf{ if } \tilde{c} \neq \emptyset \textbf{ then } \sigma\left(c\right) := \sigma\left(c\right) \cup \{\tilde{c}\}; \\ & \textbf{end;} \\ & \textbf{ if } c \neq \emptyset \textbf{ then begin} \\ & T_{\ell} := T_{\ell} \cup \{c\} \, ; \quad \text{REF}(c) = q; \quad \text{INVREF}(q) := c; \quad \text{LEVEL}(c) = \ell; \\ & \textbf{end;} \\ & \textbf{end;} \end{array}
```

Comment: Clusters having only one son or too small radius are absorbed in a neighbouring cluster;

for all $c \in T_{\ell}$ do begin

compute b(c) as the minimal box containing $\bigcup_{\tilde{c} \in \sigma(c)} b(\tilde{c})$, the approximate cluster centre \tilde{M}_c ; the approximate cluster radius $\tilde{\rho}_c$;

and the maximal side length s_c of b(c);

if $\sharp \sigma\left(c\right)=1$ or $s_c\leq c_{\min}2^{-\ell}$ then begin³

$$\mathcal{N}\left(c\right) := \left\{ \tilde{c} \in T_{\ell} \mid c \subset \mathcal{L}_{\ell+1}^{1}\left(q_{\tilde{c}}\right) \right\}; \tag{39}$$

if $\mathcal{N}\left(c\right)\neq\emptyset$ then determine $\tilde{c}\in\mathcal{N}\left(c\right)$ so that

$$s_{\tilde{c}} \geq s_{c'}, \qquad \forall c' \in \mathcal{N}\left(c\right);$$

$$T_{\ell} := T_{\ell} \setminus \{c\}; \qquad \tilde{c} := \tilde{c} \cup c; \qquad \sigma\left(\tilde{c}\right) := \sigma\left(\tilde{c}\right) \cup \sigma\left(c\right);$$

$$\text{INVREF}q_{c} = \emptyset; \ \mathbf{update} \ b\left(\tilde{c}\right), \ \tilde{M}\left(\tilde{c}\right), \ \tilde{\rho}_{\tilde{c}}, \ \text{and} \ s_{\tilde{c}};$$

end;end;end;end;

The approximations of the cluster radii and cluster centres will be employed to check whether a pair of clusters is η -admissible. A sufficient condition is given in the next lemma.

Lemma 27 Let the approximate cluster centre, radius and ball be as in the procedure **build_cluster_tree**. Let $c_1, c_2 \in T$ and put, for i = 1, 2, $\tilde{\rho}_i := \tilde{\rho}_{c_i}$ and $\tilde{B}_i := \tilde{B}(c_i)$. Then, the condition

$$\max \{\tilde{\rho}_1, \tilde{\rho}_2\} \le \eta \operatorname{dist} \left(\tilde{B}_1, \tilde{B}_2\right), \tag{40}$$

implies that the block (c_1, c_2) is η -admissible.

³We employ the notation, that, for a cluster c, the reference cube is denoted by $q_c := \text{REF}(c)$ and, for a cube $q \in \mathcal{Q}_{\ell}$, the pullback by $c_q := \text{INVREF}(c)$.

Proof. Let $i \in \{1, 2\}$. Our construction directly implies that the minimal ball B_i containing c_i is contained in \tilde{B}_i . Hence, the true cluster radii ρ_1 , ρ_2 can be estimated by

$$\max \{\rho_1, \rho_2\} \leq \max \{\tilde{\rho}_1, \tilde{\rho}_2\}.$$

Since c_i is contained in \tilde{B}_i evidently

$$\operatorname{dist}\left(\tilde{B}_{1},\tilde{B}_{2}\right)\leq\operatorname{dist}\left(c_{1},c_{2}\right).$$

We have proved that condition (40) implies

$$\max \{\rho_1, \rho_2\} \le \max \{\tilde{\rho}_1, \tilde{\rho}_2\} \le \eta \operatorname{dist} \left(\tilde{B}_1, \tilde{B}_2\right) \le \eta \operatorname{dist} \left(c_1, c_2\right)$$

and (c_1, c_2) is η -admissible.

The lemma above motivates the definition of strong η -admissibility. We employ the same notation as in that lemma.

Definition 28 A block $\mathbf{c} = (c_1, c_2) \in T^{(2)}$ is strongly η -admissible iff

$$\max \{\tilde{\rho}_1, \tilde{\rho}_2\} \le \eta \operatorname{dist} \left(\tilde{B}_1, \tilde{B}_2\right).$$

In order to check the strong η -admissibility the approximate centre and radius of the clusters have to be stored. The computation of an η -admissible, block partitioning $P^{(2)}$ of $\Gamma \times \Gamma$ is performed by using Algorithm 15, where the check of η -admissibility is replaced by checking the strong η -admissibility.

Remark 29 If the clusters along with the associated set of sons are constructed by the algorithm **build_cluster_tree**, then, T is a cluster tree.

Remark 30 For $0 \le \ell \le L$, the construction of the cluster tree implies that the tree levels

$$T(\ell) = \{c \in T \mid \text{LEVEL}(c) = \ell\}. \tag{41}$$

satisfy

$$\Gamma = \bigcup T(\ell), \quad \forall 0 \le \ell \le L,$$
 $\mathcal{G} = T(L).$

The block-cluster tree $T^{(2)}$ is determined from T (cf. Definition 13).

Remark 31 All blocks $(c_1, c_2) \in T^{(2)}$ consist of clusters of the same level:

$$LEVEL(c_1) = LEVEL(c_2)$$
.

3.2 Computation of the expansion coefficients, nearfield matrix and basis farfield coefficients

In Lemma 21, we have shown that expansion (22) has the required approximation property (Assumption 20). For the variable order panel clustering method, the expansion system (23) in (22) will be replaced by approximations to it (see Subsection 3.3) while the corresponding expansion coefficients $\overrightarrow{\kappa}_{\nu,\mu}^{(m)}(\mathbf{c})$ are as in (22). For the realization of the algorithm, they have to be computed and stored for each farfield block. Efficient algorithms for computing $\overrightarrow{\kappa}_{\nu,\mu}^{(m)}(\mathbf{c})$ are developed, for collocation discretizations, in [7] and [14] and, for Galerkin discretizations, in [8], [15], [9]. We do not recall here the details of the algorithms.

It will turn out from the error analysis that, in the special situation under consideration (discretization of an integral equation of zero order with piecewise constant elements), the nearfield matrix N can be replaced by the zero-matrix. No work at all is needed for this step.

It remains to compute the basis farfield coefficients. We consider here only the more involved case II:

$$\overrightarrow{J}_{\tau,\nu}^{II} = \int_{\tau} \overrightarrow{\Psi}_{\tau}^{(\nu)}(y) \, ds_y, \qquad \forall \nu \in \iota_{m(\tau)}^{II}, \qquad \forall \tau \in \mathcal{G}.$$

It will turn out that on the panel level, we restrict to polynomial expansions, i.e.,

$$\Phi_{\tau}^{(\nu)}(x) = (x - M_{\tau})^{\nu}, \qquad \overrightarrow{\Psi}_{\tau}^{(\nu)} = (y - M_{\tau})^{\nu} n(y).$$

In the case of flat panels, the normal vector n is constant on τ and the integration can be performed analytically (cf. [14]). For more general parametrisations, the integrals have to be evaluated numerically. Transforming τ onto the master element Q (cf. Definition 1) yields:

$$\overrightarrow{J}_{\tau,\nu}^{II} = \int_{0}^{1} \int_{0}^{\xi_{1}} g_{\tau}\left(\xi\right) \overrightarrow{\Psi}_{\tau}^{(\nu)} \circ \chi_{\tau}\left(\xi\right) d\xi,$$

where g_{τ} denotes the surface element. Since χ_{τ} and n are smooth the integrand is smooth as well. Due to (17) we know

$$|\nu| \le C_5 (m(L) + 1) \stackrel{(9)}{=} C_5 (b + 1).$$

Hence, standard quadrature formulae as, e.g., conical Gauß rules, could be applied. For given α , the number of quadrature points for conical Gauß rules approximating $J_{\tau,\nu}^{II}$ with an accuracy of $O(\operatorname{diam}^{\alpha} \tau)$ is independent of $\operatorname{diam} \tau$.

3.3 Computation of the farfield coefficients

In this subsection, we will define precisely the approximation system for the variable order panel clustering method. Before we present the formal algorithm, we start with

some motivations. We have shown that, on a cluster $c \in T$, the expansion system⁴ $\check{\Psi}_c^{(\mu,i)}=n_i\check{\Phi}_c^{(\mu)}$ (cf. 23) has the required approximation property. In order to compute the farfield coefficients $J_c^{(\mu,i)}[u]$ one has to evaluate the integrals

$$J_c^{(\mu,i)}\left[u\right] = \int_c n_i\left(y\right) \check{\Phi}_c^{(\mu)}\left(y\right) u\left(y\right) ds_y. \tag{42}$$

For the efficiency of the panel clustering method, the hierarchical structure of the cluster tree T plays a key role. The splitting of the integral

$$J_{c}^{(\mu,i)}\left[u\right] = \sum_{\tilde{c} \subset \sigma(c)} \int_{\tilde{c}} n_{i}\left(y\right) \check{\Phi}_{c}^{(\mu)}\left(y\right) u\left(y\right) ds_{y}$$

is based on this tree structure. Assume that the "consistency condition"

$$\check{\Phi}_{c}^{(\mu)} \mid_{\tilde{c}} \in \operatorname{span} \left\{ \check{\Phi}_{\tilde{c}}^{(\tilde{\mu})} : \tilde{\mu} \in \iota_{m(\tilde{c})}^{I} \right\}, \qquad \forall \mu \in \iota_{m(c)}^{I}$$

$$(43)$$

holds, i.e.,

$$\check{\Phi}_{c}^{(\mu)} \mid_{\tilde{c}} = \sum_{\tilde{\mu} \in \iota_{m}^{I}} \gamma_{\mu,\tilde{\mu},\tilde{c}} \check{\Phi}_{\tilde{c}}^{(\tilde{\mu})}. \tag{44}$$

Then, (42) can be evaluated by the recursion:

$$J_{c}^{(\mu,i)}\left[u\right] = \sum_{\tilde{c} \in \sigma(c)} \sum_{\tilde{\mu} \in \iota_{m(\tilde{c})}^{I}} \gamma_{\mu,\tilde{\mu},\tilde{c}} J_{\tilde{c}}^{(\tilde{\mu},i)}\left[u\right]$$

yielding a fast tree algorithm. Since $\check{\Phi}_c^{(\mu)}$ are polynomials, the restrictions $\check{\Phi}_c^{(\mu)}|_{\tilde{c}}$ are polynomials as well and (43) holds provided $\iota^{I}_{m(c)} \subset \iota^{I}_{m(\tilde{c})}$. Some algebraic manipulation yields that, in this case, the coefficients $\gamma_{\mu,\tilde{\mu},\tilde{c}}$ in (44) are given by

$$\gamma_{\mu,\tilde{\mu},\tilde{c}} := \begin{cases} \binom{\mu}{\tilde{\mu}} \left(M_{\tilde{c}} - M_c \right)^{\mu - \tilde{\mu}} & \tilde{\mu} \le \mu, \\ 0 & \text{otherwise.} \end{cases}$$
 (45)

For the variable order panel clustering algorithm, the expansion order m(c) satisfies

(9) resulting in $\iota^{I}_{m(c)} \not\subset \iota^{I}_{m(\tilde{c})}$ and, in general, (43) is violated.

This is the reason why we modify the expansion system for the variable order panel clustering. The system $\Phi^{(\mu)}_{c}$ should satisfy the consistency condition and have the same approximation property as the polynomials $\check{\Phi}_c^{(\mu)}$. On the panel level we put $\Phi_{\tau}^{(\mu)} = \check{\Phi}_{\tau}^{(\mu)}$, while on the larger cluster, the consistency condition (44) with $\gamma_{\mu,\tilde{\mu},\tilde{c}}$ as in (45) is explicitly used as the recursive definition of $\Phi_c^{(\mu)}$.

⁴The same arguments apply to the function system $\check{\Phi}_c^{(\nu)}$.

Definition 32 The index sets ι_m^I , ι_m^{II} , \mathbf{I}_m are given by

$$\iota_{m}^{I} : = \iota_{m}^{II} := \left\{ \nu \in \mathbb{N}_{0}^{3} \mid |\nu| \leq m \right\},
\mathbf{I}_{m} : = \left\{ (\nu, \mu) \in \mathbb{N}_{0}^{3} \times \mathbb{N}_{0}^{3} : |\nu| + |\mu| \leq m \right\}$$
(46)

and the expansion functions $\Phi_c^{(\nu)}$, $\overline{\Psi}_c^{(\nu)}$ by the recursion:

• for the panels $\tau \in \mathcal{G}$:

$$\Phi_{\tau}^{(\nu)}(x) = (x - M_{\tau})^{\nu} \quad \forall \nu \in \iota_{m(\tau)}^{I},
\overrightarrow{\Psi}_{\tau}^{(\nu)} = (y - M_{\tau})^{\nu} n(y) \quad \forall \nu \in \iota_{m(\tau)}^{II}, \tag{47}$$

• for the clusters $c \in T \backslash \mathcal{G}$:

$$\Phi_{c}^{(\nu)}|_{\widetilde{c}} = \sum_{\widetilde{\nu} \in \iota_{m(\widetilde{c})}^{I}} \gamma_{\nu,\widetilde{\nu},\widetilde{c}} \Phi_{\widetilde{c}}^{(\widetilde{\nu})} \quad \forall \nu \in \iota_{m(c)}^{I} \quad \forall \widetilde{c} \in \sigma(c),
\overrightarrow{\Psi}_{c}^{(\nu)}|_{\widetilde{c}} = \sum_{\widetilde{\nu} \in \iota_{m(\widetilde{c})}^{II}} \gamma_{\nu,\widetilde{\nu},\widetilde{c}} \overrightarrow{\Psi}_{\widetilde{c}}^{(\widetilde{\nu})} \quad \forall \nu \in \iota_{m(c)}^{II} \quad \forall \widetilde{c} \in \sigma(c).$$
(48)

Remark 33 Since the functions $\Phi_c^{(\nu)}$, $\overline{\Psi}_c^{(\nu)}$ are defined separately for each son $\tilde{c} \in \sigma(c)$, they are, in general, discontinuous. On each panel $\tau \subset c$, they are polynomials of degree b (cf. (9)). $\Phi_c^{(\nu)}$ can be regarded as an approximation to the polynomial $\Phi_c^{(\nu)} = (x - M_c)^{\nu}$ by piecewise polynomials of degree b.

Notation 34 Due to (46) we skip the superscript I, II in $\iota_{m(c)}^{I,II}$. Furthermore, we write ι_c short for $\iota_{m(c)}$ and, for a block $\mathbf{c} \in F$, $\iota_{\mathbf{c}}$ short for $\iota_{m(\mathbf{c})}$ (cf. Definition 16).

For the computation of the farfield coefficients, the hierarchical definition of the expansion functions is used. The initial step is performed on the panel level \mathcal{G} . Compute and store, for all $\tau \in \mathcal{G}$:

$$\overrightarrow{J}_{\tau,\nu}^{II}[u] := u(\tau) \overrightarrow{J}_{\tau,\nu}^{II}, \qquad \forall \nu \in \iota_{\tau}.$$

Assume inductively that all coefficients $\overrightarrow{J}_{\tilde{c},\nu}^{II}[u]$ are computed for all $\tilde{c} \in \sigma(c)$ and $c \in T \setminus \mathcal{G}$. Then

$$\overrightarrow{J}_{c,\nu}^{II}\left[u\right] = \int_{c} \overrightarrow{\Psi}_{c}^{(\nu)}\left(y\right) u\left(y\right) ds_{y} = \sum_{\widetilde{c} \in \sigma(c)} \int_{\widetilde{c}} \overrightarrow{\Psi}_{c}^{(\nu)}\left(y\right) u\left(y\right) ds_{y}, \qquad \forall \nu \in \iota_{c}.$$

By using (48) we obtain

$$\overrightarrow{J}_{c,\nu}^{II}[u] = \sum_{\widetilde{c}\in\sigma(c)} \sum_{\widetilde{\nu}\in\iota_{\widetilde{c}}} \gamma_{\nu,\widetilde{\nu},\widetilde{c}} \overrightarrow{J}_{\widetilde{c},\widetilde{\nu}}^{II}[u], \qquad \forall \nu \in \iota_{c}.$$
(49)

3.4 Evaluation of a matrix vector multiplication

The computation of the quantities $A_{\mathbf{c},\nu}[u]$ is straightforward. It will turn out that it is preferable to compute and store directly the quantities⁵:

$$B_{c_1}^{(\nu)}[u] := \sum_{c_2:(c_1,c_2)\in F} \tilde{A}_{\mathbf{c}}^{(\nu)}[u], \qquad \forall c_1 \in T, \qquad \forall \nu \in \iota_{c_1}$$
 (50)

with

$$\tilde{A}_{\mathbf{c}}^{(\nu)}[u] := \begin{cases} A_{\mathbf{c}}^{(\nu)}[u], & \text{if } \nu \in \iota_{\mathbf{c}}, \\ 0 & \text{if } \nu \in \iota_{c_1} \setminus \iota_{\mathbf{c}}, \end{cases} \quad \forall \mathbf{c} = (c_1, c_2) \in F.$$

We turn to the evaluation of the sum in (30). Since we replaced the nearfield matrix N by the zero, the sum in (30) consists only of the farfield evaluation:

$$\mathbf{v}_{\tau} = \sum_{\mathbf{c} \in F} \sum_{\nu \in I_{\mathbf{c}}} \int_{c_{1}} A_{\mathbf{c}}^{(\nu)} \left[u \right] \Phi_{c_{1}}^{(\nu)} \left(x \right) b_{\tau} \left(x \right) ds_{x}. \tag{51}$$

In view of (50), it is advantageous to rewrite this formula as

$$\mathbf{v}_{\tau} = \sum_{c_1 \in T} \sum_{\nu \in \iota_{c_1}} \int_{c_1} B_{c_1}^{(\nu)} [u] \Phi_{c_1}^{(\nu)} (x) b_{\tau} (x) ds_x.$$
 (52)

In the next step, we will derive a hierarchical representation of this formula. The summation over $c_1 \in T \setminus \mathcal{G}$ in (52) can be split into a sum over the sons $\sigma(c_1)$. We obtain

$$\sum_{\nu \in \iota_{c_{1}}} \int_{c_{1}} B_{c_{1}}^{(\nu)} \left[u \right] \Phi_{c_{1}}^{(\nu)} \left(x \right) b_{\tau} \left(x \right) ds_{x} = \sum_{\widetilde{c}_{1} \in \sigma(c_{1})} \sum_{\nu \in \iota_{c_{1}}} \int_{\widetilde{c}_{1}} B_{c_{1}}^{(\nu)} \left[u \right] \Phi_{c_{1}}^{(\nu)} \left(x \right) b_{\tau} \left(x \right) ds_{x}.$$
 (53)

On the other hand, the summation in (52) contains a partial sum over $\sigma(c_1)$ of the form:

$$\sum_{\widetilde{c_1} \in \sigma(c_1)} \sum_{\widetilde{\nu} \in \iota_{\widetilde{c_1}}} \int_{\widetilde{c_1}} B_{\widetilde{c_1}}^{(\widetilde{\nu})} \left[u \right] \Phi_{\widetilde{c_1}}^{(\widetilde{\nu})} \left(x \right) b_{\tau} \left(x \right) ds_x. \tag{54}$$

In the next step, the right-hand side in (53) will be added to (54). Plugging in (48) into (53) and re-organizing the terms shows that the sum in (53) equals

$$\sum_{\widetilde{c_{1}} \in \sigma(c_{1})} \sum_{\widetilde{\nu} \in \iota_{\widetilde{c_{1}}}} \int_{\widetilde{c_{1}}} R_{\widetilde{c_{1}}}^{(\widetilde{\nu})} \left[u\right] \Phi_{\widetilde{c_{1}}}^{(\widetilde{\nu})} \left(x\right) b_{\tau} \left(x\right) ds_{x}$$

with

$$R_{\widetilde{c_1}}^{(\widetilde{\nu})}[u] = \sum_{\nu \in \iota_{c_1}} \gamma_{\nu, \widetilde{\nu}, \widetilde{c_1}} B_{c_1}^{(\nu)}[u].$$

Frecall that, for $\mathbf{c} = (c_1, c_2) \in F$, we have $m(c_1) \ge m(\mathbf{c})$ (cf. (35), (18)) implying $\iota_{m(\mathbf{c})}^I \subset \iota_{m(c_1)}^I$)

Hence, (53) and (54) can be added resulting in

$$\sum_{\widetilde{c_{1}} \in \sigma(c_{1})} \sum_{\widetilde{\nu} \in \iota_{\widetilde{c_{1}}}} \int_{\widetilde{c_{1}}} \left(R_{\widetilde{c_{1}}}^{(\widetilde{\nu})} \left[u \right] + B_{\widetilde{c_{1}}}^{(\widetilde{\nu})} \left[u \right] \right) \Phi_{\widetilde{c_{1}}}^{(\widetilde{\nu})} \left(x \right) b_{\tau} \left(x \right) ds_{x}.$$

Iterating this algorithms over the hierarchical structure of T leads to Algorithm 35 for the evaluation of \mathbf{v}_{τ} . The tree levels $T(\ell)$ are as in Definition 10 and $B_c^{(\nu)}[u]$ as in (50).

Algorithm 35 The procedure **evaluate_sums** shifts the expansions from the coarse levels to the finer ones and accumulates the coefficients on the finest level.

```
\begin{array}{l} \textit{procedure evaluate\_sum;begin} \\ \textit{for all } \nu \in \iota_{\Gamma} \textit{ do } \mathcal{R}_{\Gamma}^{(\nu)}[u] := B_{\Gamma}^{(\nu)}[u] \,; \\ \textit{for all } \ell := 0 \textit{ to } L - 1 \textit{ do} \\ \textit{ for all } c \in T(\ell) \textit{ do} \\ \textit{ for all } \widetilde{c} \in \sigma\left(c\right) \textit{ do begin for all } \widetilde{\nu} \in \iota_{\widetilde{c}} \\ \mathcal{R}_{\widetilde{c}}^{(\widetilde{\nu})}[u] := B_{\widetilde{c}}^{(\widetilde{\nu})}[u] + \sum_{\nu \in \iota_{c}} \gamma_{\nu,\widetilde{\nu},\widetilde{c}} \mathcal{R}_{c}^{(\nu)}[u] \,; \\ \textit{end;} \\ \textit{for all } \tau \in \mathcal{G} \textit{ do} \\ \\ \mathbf{v}_{\tau} := \sum_{\nu \in \iota_{\tau}} \mathcal{R}_{\tau}^{(\nu)}[u] J_{\tau,\nu}^{I}; \\ \textit{end;} \\ \\ \textit{end;} \end{array}
```

4 Error analysis

4.1 Abstract error estimates

We have presented a variable order panel clustering algorithm based on block partitionings of $\Gamma \times \Gamma$ for the discretization of the second kind integral equation in (1). The discretization is based on piecewise constant finite element spaces. It is well known in the theory of boundary elements that the Galerkin solution to this problem converges as

$$||u - u_G||_{0,\Gamma} \le Ch ||f||_{1,\Gamma} \tag{55}$$

provided $f \in H^1(\Gamma)$ where $\|\cdot\|_{1,\Gamma}$ denotes the H^1 -norm. Let $\widetilde{u_G} \in S^{-1,0}$ denote the solution if the integral operator in (3) is replaced by the panel clustering approximation. In this section, we will prove that, under the abstract Assumption 20, the solution $\widetilde{u_G}$ exists and satisfies the error estimate (55), too, with a possibly larger constant C. In this section, the error estimates will be derived from abstract assumptions while, in Sections 4.2 and 4.3, we will show that these assumptions are satisfied for shape regular, quasi-uniform meshes.

Definition 36 The uniformity of a mesh \mathcal{G} is characterized by the smallest constant C_u satisfying

$$h \le C_u h_{\tau}, \quad \forall \tau \in \mathcal{G}$$

where h is as in (32) and

$$h_{\tau} := \operatorname{diam} \tau.$$

Definition 37 The quality of panels is characterized by the smallest constant C_q satisfying

$$h_{\tau}^2 \le C_q |\tau|, \quad \forall \tau \in \mathcal{G}.$$

Remark 38 Since \mathcal{G} only contains finitely many panels, the constants C_u, C_q are always bounded. However, it will turn out that the constants in the estimates below behaves critically with increasing values of C_q , C_u and we assume here that C_q and C_u are of moderate size.

Assumption 39 The tree T is balanced in the sense that all panels $\tau \in \mathcal{G}$ have the same depth in the tree:

LEVEL
$$(\tau) = L$$
, $\forall \tau \in \mathcal{G}$.

Remark 40 By using the construction of Subsection 3.1, Assumption 39 is always guaranteed.

Remark 41 Definition 13 and 14 imply that all blocks $\mathbf{c} = (c_1, c_2) \in P^{(2)}$ consist of clusters of the same level:

LEVEL
$$(c_1)$$
 = LEVEL (c_2) .

For $0 \le \ell \le L$, we introduce the farfield levels $F(\ell)$ by

$$F(\ell) = \{(c_1, c_2) \in F : \text{LEVEL}(c_1) = \text{LEVEL}(c_2) = \ell\}.$$

Then, the function $m: F \to \mathbb{N}_0$ as in Definition 16 only depends on the level ℓ . For $\mathbf{c} \in F(\ell)$, we have

$$m\left(\mathbf{c}\right) = a\left(L - \ell\right) + b. \tag{56}$$

The right-hand side in (56) defines a function $\tilde{m}: \mathbb{N}_0 \to \mathbb{N}_0$. If there is no ambiguity we write again m instead of \tilde{m} .

Assumption 42 There exist constants $C_6 < \infty$ and $1 < C_7 < \infty$ so that, for all $0 \le \ell \le L$ and any $c \in T(\ell)$:

$$C_7^{-1}2^{-\ell} \leq \rho_c \leq C_7 2^{-\ell},$$

$$\operatorname{diam} c \leq C_6 h 2^{L-\ell}.$$

Assumption 43 The constants a in (9) is chosen so that a > 1 and $2C_2^a =: C_8 < 1$ holds with C_2 as in Assumption 20.

We need an assumption estimating, for $c_1 \in T(\ell)$, the number of clusters c_2 forming a block (c_1, c_2) in $F(\ell)$.

Assumption 44 There exist positive constants C_9^I , $C_9^{II} < \infty$ so that, for all $0 \le \ell \le L$ and all $c \in T(\ell)$:

$$\sharp \left\{ \mathbf{c} \in F\left(\ell\right) : c_1 = c \right\} \leq C_9^I,$$

$$\sharp \left\{ \mathbf{c} \in F\left(\ell\right) : c_2 = c \right\} \leq C_9^{II}.$$

The nearfield matrix is replaced by zero. In order to estimate the arising error we need an assumption concerning the number of nearfield matrix entries.

Assumption 45 There exist positive constants C_{10}^I , C_{10}^{II} < ∞ so that, for all $0 \le \ell \le L$ and all $\tau \in \mathcal{G}$:

$$\sharp \{ t \in \mathcal{G} : (\tau, t) \in N \} \leq C_{10}^{I},$$

$$\sharp \{ t \in \mathcal{G} : (t, \tau) \in N \} < C_{10}^{II},$$

with N as in (8).

The error estimate of the Galerkin discretization including panel clustering is based on the second Strang lemma [1]. For $u, v \in S^{-1,0}$, let

$$E := \left| \left(v, K\left[u \right] - \widetilde{K}\left[u \right] \right) \right|,$$

where \tilde{K} denotes the panel clustering approximation to K. In order to estimate E, we need an auxiliary result.

Lemma 46 Let Assumption 20, 39, and 42 be satisfied. There exists a constant $C_{11} < \infty$ so that, for all $0 \le \ell \le L$ and every $\mathbf{c} \in F(\ell)$

$$\sqrt{|c_1| |c_2|} C_2^{m(\ell)} \operatorname{dist}^{-1}(c_1, c_2) \le C_{11} h C_8^{L-\ell}.$$
(57)

Proof. Recall that $0 \leq C_2 < 1$. Let $\mathbf{c} \in F(\ell)$. Without loss of generality we assume that

$$\rho_{c_1} = \max \{ \rho_{c_1}, \rho_{c_2} \} .$$

Hence,

$$\sqrt{|c_1|\,|c_2|} \le C\rho_{c_1}^2,$$

where C depends only on (the curvature of) the surface Γ . Using (7), Assumptions 42 and 39 we obtain

$$\sqrt{|c_1||c_2|}C_2^{m(\ell)}\operatorname{dist}^{-1}(c_1,c_2) \le C\eta\rho_{c_1}C_2^{m(\ell)} \le CC_6h2^{L-\ell}C_2^{m(\ell)}$$

and, by employing Assumption 43,

$$\sqrt{|c_1||c_2|}C_2^{m(\ell)}\operatorname{dist}^{-1}(c_1,c_2) \le CC_6h(2C_2^a)^{L-\ell} = CC_6hC_8^{L-\ell}$$

Lemma 47 Let Assumptions 20, 39, 42, 43, 44, and 45 be satisfied. There exists a constant C so that, for all $u, v \in S^{-1,0}$:

$$E \le Ch \|u\|_{0,\Gamma} \|v\|_{0,\Gamma}.$$

Proof. We employ the splitting $E = E_1 + E_2$ with

$$E_{1} = \sum_{\ell=0}^{L} \sum_{\mathbf{c} \in F(\ell)} \int_{\mathbf{c}} u(x) v(y) \left(k(x,y) - k_{\mathbf{c}}^{m(\ell)}(x,y) \right) ds_{y} ds_{x}$$

$$E_{2} = \sum_{(t,\tau) \in N} \int_{t \times \tau} u(x) v(y) k(x,y) ds_{y} ds_{x}$$

and estimate E_1 , E_2 separately.

$$\begin{split} E_{1} &\leq \sum_{\ell=0}^{L} \sum_{\mathbf{c} \in F(\ell)} \int_{\mathbf{c}} |u\left(x\right)| \left|v\left(y\right)\right| \left|k\left(x,y\right) - k_{\mathbf{c}}^{m(\ell)}\left(x,y\right)\right| ds_{y} ds_{x} \\ &\stackrel{(11)}{\leq} \sum_{\ell=0}^{L} \sum_{\mathbf{c} \in F(\ell)} \sqrt{\left|c_{1}\right| \left|c_{2}\right|} C_{1} C_{2}^{m(\ell)} \operatorname{dist}^{-1}\left(c_{1},c_{2}\right) \left\|u\right\|_{0,c_{1}} \left\|v\right\|_{0,c_{2}} \\ &\stackrel{(57)}{\leq} C_{11} C_{1} h \sum_{\ell=0}^{L} C_{8}^{L-\ell} \sum_{\mathbf{c} \in F(\ell)} \left\|u\right\|_{0,c_{1}} \left\|v\right\|_{0,c_{2}} \\ &\leq C_{11} C_{1} h \sum_{\ell=0}^{L} C_{8}^{L-\ell} \left\{ \sum_{\mathbf{c} \in F(\ell)} \left\|u\right\|_{0,c_{1}}^{2} \right\}^{1/2} \left\{ \sum_{\mathbf{c} \in F(\ell)} \left\|v\right\|_{0,c_{2}}^{2} \right\}^{1/2} \\ &\leq C_{11} C_{1} h \sum_{\ell=0}^{L} C_{8}^{L-\ell} \left\{ \sum_{c_{1} \in T(\ell)} \left\|u\right\|_{0,c_{1}}^{2} \sum_{c_{2}: \mathbf{c} \in F(\ell)} 1 \right\}^{1/2} \left\{ \sum_{c_{2} \in T(\ell)} \left\|v\right\|_{0,c_{2}}^{2} \sum_{c_{1}: \mathbf{c} \in F(\ell)} 1 \right\}^{1/2} \\ &\leq C_{11} C_{1} \sqrt{C_{9}^{I} C_{9}^{II}} h \left\|u\right\|_{0,\Gamma} \left\|v\right\|_{0,\Gamma} \sum_{\ell=0}^{L} C_{8}^{L-\ell} \leq \frac{C_{11} C_{1} \sqrt{C_{9}^{I} C_{9}^{II}}}{1 - C_{8}} h \left\|u\right\|_{0,\Gamma} \left\|v\right\|_{0,\Gamma} . \end{split}$$

For the estimate of E_2 we begin with considering a single pair of panels $(t, \tau) \in N$:

$$\left| \int_{t} v(x) \int_{\tau} u(y) k(x,y) \right| ds_{y} ds_{x} \leq C_{\Gamma} \int_{t} |v(x)| dx \int_{\tau} |u(y)| \|x - y\|^{-1} ds_{y} ds_{x}$$

$$\leq C_{\Gamma} \|v\|_{\infty,t} \|u\|_{\infty,\tau} \int_{t \times \tau} \|x - y\|^{-1} ds_{y} ds_{x}. \tag{58}$$

Since u is constant on t and v on τ , we get

$$||v||_{\infty,t} ||u||_{\infty,\tau} = \frac{||v||_{0,t} ||u||_{0,\tau}}{\sqrt{|t||\tau|}}.$$

We turn to the integral in (58). We distinguish two cases:

(a) dist $(\tau, t) > 0$. The shape regularity and the quasi-uniformity of the meshes imply:

$$\operatorname{dist}(\tau, t) \geq Ch$$
.

Hence.

$$||v||_{\infty,t} ||u||_{\infty,\tau} \int_{t \le \tau} ||x-y||^{-1} ds_y ds_x \le C^{-1} h^{-1} \sqrt{|t| |\tau|} ||v||_{0,t} ||u||_{0,\tau} \le C^{-1} h ||v||_{0,t} ||u||_{0,\tau}.$$

(b) dist $(\tau, t) = 0$. There exists a mapping $\chi : \mathbb{R}^2 \to \mathbb{R}^3$ which is sufficiently smooth, independent of h along with a subset $\mathcal{U} \subset \mathbb{R}^2$ with $\chi(\mathcal{U}) = t \cup \tau$. Furthermore, we may assume that there exists a constant C independent of h so that \mathcal{U} is contained in a ball B centred at the origin with radius Ch. Then,

$$\int_{t \times \tau} \|x - y\|^{-1} ds_y ds_x \le C \int_{B \times B} \|\chi(\xi) - \chi(\theta)\|^{-1} d\theta d\xi.$$

We introduce polar coordinates at ξ :

$$\theta = \xi + r\psi(\alpha)$$

with $\psi(\alpha) = (\cos \alpha, \sin \alpha)^{\mathsf{T}}$. Hence,

$$\int_{t \times \tau} \|x - y\|^{-1} ds_y ds_x \le C \int_B \int_0^{Ch} \int_0^{2\pi} r \|\chi(\xi) - \chi(\xi + r\psi)\|^{-1} d\alpha dr d\xi.$$

The quotient

$$\frac{r}{\|\chi\left(\xi\right) - \chi\left(\xi + r\psi\right)\|}$$

stays bounded as $r \to 0$ as a consequence of the regularity of Γ . Thus,

$$\int_{t \times \tau} \|x - y\|^{-1} ds_y ds_x \le C \int_B \int_0^{Ch} \int_0^{2\pi} 1 d\alpha dr d\xi \le Ch^3,$$
$$\|v\|_{\infty,t} \|u\|_{\infty,\tau} \int_{t \times \tau} \|x - y\|^{-1} ds_y ds_x \le Ch \|v\|_{0,t} \|u\|_{0,\tau}.$$

Summing all nearfield entries yields:

$$E_{2} \leq Ch \sum_{(t,\tau)\in N} \|v\|_{0,t} \|u\|_{0,\tau} \leq Ch \left\{ \sum_{(t,\tau)\in N} \|v\|_{0,t}^{2} \right\}^{1/2} \left\{ \sum_{(t,\tau)\in N} \|u\|_{0,\tau}^{2} \right\}^{1/2}$$

$$\leq Ch \left\{ \sum_{t\in\mathcal{G}} \|v\|_{0,t}^{2} \sum_{\tau:(t,\tau)\in N} 1 \right\}^{1/2} \left\{ \sum_{\tau\in\mathcal{G}} \|u\|_{0,\tau}^{2} \sum_{t:(t,\tau)\in N} 1 \right\}^{1/2} \leq C\sqrt{C_{10}^{I}C_{10}^{II}} h \|v\|_{0,\Gamma} \|u\|_{0,\Gamma}.$$

Theorem 48 Let the assumptions of Lemma 47 be satisfied and h sufficiently small. Then, the solution $\widetilde{u_G}$ to (3) with K replaced by the panel clustering approximation exists for any $f \in L^2(\Gamma)$. If $f \in H^1(\Gamma)$ the error estimate

$$\|u - \widetilde{u_G}\|_{0,\Gamma} \le Ch \|f\|_{1,\Gamma}$$

holds.

Proof. In view of Lemma 47 the result follows from [1, Lemma 4.1.1]. ■

4.2 Verifying the assumptions on the cluster tree and the partitioning $P^{(2)}$

In this subsection, the abstract geometric Assumptions 42, 44, and 45 are proved for shape regular, quasi-uniform meshes. In [7], related results have been proved by formulating certain abstract assumptions (see [7, Criterion (B.1 d), (B.7)]) for the cluster tree. Then, it was shown that surface meshes being images of Cartesian grids in the parameter plane satisfy these assumptions. Our construction (procedure **build_cluster_tree**) applies for any quasi-uniform surface mesh while the analysis is different from [7].

We impose two further geometric assumptions on the surface Γ : The first one is satisfied for all reasonable surfaces and the second one is imposed to reduce technicalities.

Notation 49 The three dimensional ball (with respect to the maximum norm) centred at $x \in \mathbb{R}^3$ with radius r is denoted by $B_r^{\infty}(x)$. For r > 0, the r-neighbourhood of Γ is

$$U_r\left(\Gamma\right) := \left\{x \in \mathbb{R}^3 \mid \exists y \in \Gamma : ||x - y|| \le r\right\}.$$

Assumption 50 There exist positive constants c_{Γ} , C_{Γ} so that, for all $x \in \Gamma$ and all $0 < r < \operatorname{diam} \Gamma$

$$|B_r^{\infty}(x) \cap \Gamma| \geq c_{\Gamma} r^2,$$

$$|U_r(\Gamma)| < C_{\Gamma} r.$$

For all subsets $\gamma \subset \Gamma$, the diameter diam γ can be estimated by

$$\operatorname{diam} \gamma \geq c_{\Gamma} \sqrt{|\gamma|},$$

where $|\gamma|$ denotes the two-dimensional surface measure of γ .

Assumption 51 Γ *is a closed, simply connected surface.*

Lemma 52 Let Assumption 50 and 51 be satisfied. Let $\ell \leq L - \delta$ with $\delta := \text{lb}\left(16\sqrt{3}C_u\right)$. In procedure **build_cluster_tree** choose $c_{\min} \leq \min\left\{4, \sqrt{c_{\Gamma}^3/2}\right\}/32$. Assume $c \in T(\ell)$ satisfies

$$s_c < c_{\min} 2^{-\ell}$$
.

Then, there exists $\check{c} \in T(\ell)$ (with reference cluster $\check{q} := \text{REF}(\check{c})$) satisfying (cf. (26)):

$$c \subset \mathcal{L}^1_{\ell+1}(\check{q}), \qquad s_{\check{c}} \geq c_{\min} 2^{-\ell}.$$

Proof. We may assume that $\ell > 0$ since, for $\ell = 0$, we have $c = \Gamma$ and $s_{\Gamma} = 1 \ge c_{\min}$. Let $c \in T(\ell)$ with $\ell \le L - \delta$ (δ as above). Put $q_c := \text{REF}(c)$. Since Γ is closed (cf. Assumption 51) there exists $\tau \in \mathcal{G}$ with $\overline{\tau} \cap \overline{c} \ne \emptyset$ and $\tau \cap c = \emptyset$. Hence, $\tau \cap \partial q \ne \emptyset$ implying

$$\operatorname{dist}(\partial q, c) \leq h.$$

Choose $x \in \tau$ (implying $x \in \Gamma$). Hence, $c \in B_{r_1}^{\infty}(x)$ (cf. Notation 49) with $r_1 = h + s_c$. Condition (35) and Definition 36 imply:

$$r_1 \le 2\sqrt{3}C_u 2^{-L} + c_{\min} 2^{-\ell} = 2^{-\ell-2} \left(8\sqrt{3}C_u 2^{\ell-L} + 4c_{\min} \right) \le 2^{-\ell-2}.$$
 (59)

Now, consider $B_{r_2}^{\infty}\left(x\right)$ with $r_2=2^{-\ell-3}$ and put $\gamma=\Gamma\cap B_{r_2}^{\infty}\left(x\right)$. Denote

$$\mathcal{G}\left(\gamma\right):=\left\{ au\in\mathcal{G}: au\cap\gamma\neq\emptyset
ight\} .$$

Hence, all approximate cluster centres of $\tau \in \mathcal{G}(\gamma)$ are contained in $B_{r_3}^{\infty}(x)$ with $r_3 = 2^{-\ell-3} + h$. Similarly to the estimate of r_1 in (59) one derives $r_3 \leq 2^{-\ell-2}$. Define

$$\mathcal{N}\left(x\right) := \left\{ \tilde{q} \in \mathcal{Q}_{\ell} \mid B_{r_{3}}^{\infty}\left(x\right) \cap \tilde{q} \neq \emptyset \right\}.$$

Then, all $\tilde{q} \in \mathcal{N}(x)$ have the property $b_c \subset \mathcal{L}^1_{\ell+1}(\tilde{q})$. Assumption 50 implies that

$$\left| \bigcup_{\tilde{q} \in \mathcal{N}(x)} \text{INVREF} \left(\tilde{q} \right) \right| \ge \left| B_{r_2}^{\infty} \left(x \right) \cap \Gamma \right| \ge c_{\Gamma} r_2^2$$

holds. Obviously, $\sharp \mathcal{N}(x) \leq 8$ and, hence, there exists $\tilde{q} \in \mathcal{N}(x)$ with associated cluster $\tilde{c} := \text{INVREF}(\tilde{q})$ satisfying $|\tilde{c}| \geq r_2^2 c_{\Gamma}/8$. By using Assumption 50 we obtain:

$$s_{\tilde{c}} \ge \rho_{\tilde{c}} \ge \frac{1}{2} \operatorname{diam} \tilde{c} \ge \frac{1}{2} c_{\Gamma} \sqrt{|\tilde{c}|} \ge \frac{1}{2\sqrt{8}} c_{\Gamma} r_2 \sqrt{c_{\Gamma}} = \frac{c_{\Gamma}^{3/2}}{32\sqrt{2}} 2^{-\ell} \ge c_{\min} 2^{-\ell}.$$

In view of this Lemma we formulate the assumption concerning the choice of c_{\min} .

Assumption 53 The constant c_{\min} in the procedure **build_cluster_tree** is chosen so that

$$c_{\min} \le \min \left\{ 4, \sqrt{c_{\Gamma}^3/2} \right\} / 32.$$

Lemma 54 Let the cluster tree be generated by the procedure **build_cluster_tree**. Let Assumption 50, 51, and 53 be satisfied. Then, there exist constants $C_6 < \infty$ and $1 \le C_7 < \infty$ so that, for all $0 \le \ell \le L$ and every $c \in T(\ell)$:

$$C_7^{-1}2^{-\ell} \le \rho_c \le C_7 2^{-\ell}$$
 (60)

$$\operatorname{diam} c \leq C_6 h 2^{L-\ell}. \tag{61}$$

Proof. (a) The largest cluster $c = \Gamma$ clearly satisfies (60) and we may restrict to the case $c \neq \Gamma$.

(b) We first prove the left-hand side in (60). Lemma 52 implies that, for all $\ell \leq L - \delta$, the procedure **build_cluster_tree** guarantees

$$s_c \ge c_{\min} 2^{-\ell}, \quad \forall c \in T(\ell).$$

For the cluster radius we obtain

$$\rho_c \ge \frac{1}{2} \operatorname{diam} c \ge s_c/2 \ge \left(\frac{1}{2}c_{\min}\right) 2^{-\ell}.$$

For $\ell > L - \delta$ and $c \in T(\ell)$ we obtain with ρ as in (31)

$$\rho_c \ge \underline{\rho} \ge \sqrt{3} \frac{h_L}{2} = \left(\frac{1}{2} \sqrt{3} 2^{\ell - L}\right) 2^{-\ell} \ge \left(\frac{1}{2} \sqrt{3} 2^{-\delta}\right) 2^{-\ell} = \left(\frac{1}{32C_u}\right) 2^{-\ell}.$$

(c) Next, we will prove the right-hand side in (60). First, we will show that any $c \in T(\ell)$ is contained in

$$\mathcal{L}_{L}^{d}\left(\mathcal{L}_{L-1}^{1}\left(\mathcal{L}_{L-2}^{1}\left(\ldots\left(\mathcal{L}_{\ell+1}^{1}\left(q_{c}\right)\right)\right)\right)\right)$$

with $q_c := \text{REF}(c)$ and $d = \lceil 2\sqrt{3}C_u \rceil$.

The proof of this assertion is given by induction with respect to ℓ .

• $\ell = L$. Then, $T(L) = \mathcal{G}$. Choose $\tau \in T(L)$ and put $q := \text{REF}(\tau)$. The side length of q is h_L . Let $t \in \mathcal{G}$ so that $\rho_t = \underline{\rho}$ holds (cf. (35)). Due to (35) we know

$$\rho_{\tau} \le h_{\tau} \le C_u h_t \le 2C_u \rho \le 2\sqrt{3}C_u h_L$$

and, hence, τ is contained in $\mathcal{L}_L^d(q)$ with $d = \lceil 2\sqrt{3}C_u \rceil$.

• Assume that the assertion holds for $k = \ell + 1, \ell + 2, \dots, L$.

• The assumption of the induction implies that each $\tilde{c} \in T(\ell+1)$ is contained in

$$\mathcal{L}_{L}^{d}\left(\mathcal{L}_{L-1}^{1}\left(\mathcal{L}_{L-2}^{1}\left(\ldots\left(\mathcal{L}_{\ell+2}^{1}\left(\widetilde{q}\right)\right)\right)\right)\right)$$

with $\tilde{q} := \text{REF}(\tilde{c})$. Since c is either not "absorbed" (cf. procedure **build_cluster_tree**) or absorbed in a cluster c' satisfying $c \subset \mathcal{L}^1_{\ell+1}(q')$ with q' := REF(c') the cluster c is contained in

$$\mathcal{L}_{L}^{d}\left(\mathcal{L}_{L-1}^{1}\left(\mathcal{L}_{L-2}^{1}\left(\ldots\left(\mathcal{L}_{\ell+1}^{1}\left(q\right)\right)\right)\right)\right). \tag{62}$$

(d) The right-hand side in (62) is a cube with side length

$$h_q + 2(h_q 2^{-1} + h_q 2^{-2} + \dots + h_q 2^{1-L} + dh_q 2^{-L}) \le 4dh_q = 4d2^{-\ell}.$$
 (63)

Hence, the cluster radius of any $c \in T(\ell)$ can be estimated by

$$\rho_c \le \operatorname{diam} c \le 4\sqrt{3}d2^{-\ell} \le \left(24C_u + 4\sqrt{3}\right)2^{-\ell}$$
(64)

and the assertion holds with $C_7 = 24C_u + 4\sqrt{3}$.

(e) The estimate (61) follows from (64) via

$$\operatorname{diam} c \leq C_7 2^{-\ell} \leq C_7 h_L 2^{L-\ell} \stackrel{(35)}{\leq} C_7 \frac{2}{\sqrt{3}} \underline{\rho} 2^{L-\ell} \leq C_7 \frac{2}{\sqrt{3}} h 2^{L-\ell} =: C_6 h 2^{L-\ell}.$$

Lemma 55 Let the Assumptions of Lemma 54 be satisfied and the construction of $P^{(2)}$ be based on the strong admissibility condition. Then, there exist positive constants C_9^I , $C_9^{II} < \infty$ so that, for all $0 \le \ell \le L$ and all $\tau \in T(\ell)$:

$$\sharp \left\{ \mathbf{c} \in F\left(\ell\right) : \tau = c_1 \right\} \le C_9^I,
\sharp \left\{ \mathbf{c} \in F\left(\ell\right) : \tau = c_2 \right\} \le C_9^{II}.$$
(65)

Proof. For $\ell = 0$, the left-hand sides in (65) are zero since $F(0) = \emptyset$ due to $T^{(2)}(0) = \{(\Gamma, \Gamma)\}$ and (Γ, Γ) is non-admissible.

Let $\ell \geq 1$ and $\tilde{c}_1 \in T(\ell)$. The father of \tilde{c}_1 is denoted by $c_1 \in T(\ell-1)$ and characterized by

$$\tilde{c}_1 \in \sigma(c_1)$$
.

Let $\tilde{c}_2 \in T(\ell)$ with $\mathbf{c} = (c_1, c_2) \in F(\ell)$. The father of \tilde{c}_2 is denoted by c_2 . Since the construction of $P^{(2)}$ was based on strong admissibility, we have

$$\max \left\{ \tilde{\rho}_{c_{1}}, \tilde{\rho}_{c_{2}} \right\} > \eta \operatorname{dist} \left(\tilde{B} \left(c_{1} \right), \tilde{B} \left(c_{2} \right) \right), \tag{66}$$

$$\max \left\{ \tilde{\rho}_{\tilde{c}_{1}}, \tilde{\rho}_{\tilde{c}_{2}} \right\} \leq \eta \operatorname{dist} \left(\tilde{B} \left(\tilde{c}_{1} \right), \tilde{B} \left(\tilde{c}_{2} \right) \right).$$

Using (33) we get

$$\operatorname{dist}\left(\tilde{B}\left(\tilde{c}_{1}\right),\tilde{B}\left(\tilde{c}_{2}\right)\right) \leq \operatorname{dist}\left(\tilde{B}\left(c_{1}\right),\tilde{B}\left(c_{2}\right)\right) + 2\tilde{\rho}_{c_{1}} + 2\tilde{\rho}_{c_{2}} \stackrel{(66)}{<} \left(2 + 1/\eta\right)\left(\tilde{\rho}_{c_{1}} + \tilde{\rho}_{c_{2}}\right).$$

The approximate $\tilde{\rho}_{c_1}$ was defined as the Čebyšev radius of the minimal cube containing c_1 . This cube is smaller than the box (62) yielding (by using (63))

$$\tilde{\rho}_{c_1} \le \sqrt{3} s_{c_1} \le 4d\sqrt{3} 2^{-\ell}$$
.

This implies that, for fixed \tilde{c}_1 , all strongly η -admissible clusters \tilde{c}_2 are contained in the ball $\mathcal{B}(c_1)$ centred at the approximate cluster centre $\tilde{z}_{\tilde{c}_1}$ with radius

$$\tilde{\rho}_{c_1} + (2 + 1/\eta) (\tilde{\rho}_{c_1} + \tilde{\rho}_{c_2}) + 2\tilde{\rho}_{c_2} \leq \tilde{C}h_{\ell}.$$

The number of clusters c_2 being strongly η -admissible with respect to c_1 is bounded by the number of cubes $q_{\ell} \in \mathcal{Q}_{\ell}$ touching $\mathcal{B}(c_1)$. Since $|\mathcal{B}(c_1)| \leq 4/3\pi \left(\tilde{C}h_{\ell}\right)^3$ and $|q_{\ell}| = h_{\ell}^3$, this number is bounded by a constant C_9^I independent of ℓ and c_1 . The estimate of $C_9^{II} \leq C'$ is just a repetition of the arguments.

Lemma 56 Let the Assumptions of Lemma 54 be satisfied and the construction of $P^{(2)}$ be based on the strong-admissibility condition. Then, there exists positive constants C_{10}^{I} , $C_{10}^{II} < \infty$ so that, for all $0 \le \ell \le L$ and all $\tau \in \mathcal{G}$

$$\sharp \{ t \in \mathcal{G} : (\tau, t) \in N \} \leq C_{10}^{I},$$

$$\sharp \{ t \in \mathcal{G} : (t, \tau) \in N \} \leq C_{10}^{II}.$$

Proof. Let $\tau \in \mathcal{G}$. Every $t \in \mathcal{G}$ with $(\tau, t) \in N$ satisfies

$$\max \{\rho_t, \rho_\tau\} > \eta \operatorname{dist}(B_t, B_\tau)$$

since, on the panel level, the cluster balls and radii are computed exactly. Hence,

$$\operatorname{dist}(t,\tau) \leq \operatorname{dist}(B_t, B_\tau) + 2\rho_t + 2\rho_\tau \leq h\left(\frac{1}{\eta} + 4\right) \leq 2\left(\frac{1}{\eta} + 4\right)C_u\underline{\rho} \leq 2\left(\frac{1}{\eta} + 4\right)C_u\sqrt{3}h_L.$$

Any $t \in \mathcal{G}$ with $(\tau, t) \in N$ is contained in a ball $\mathcal{B}(\tau)$ centred at the centre of τ with radius

$$2\left(\frac{1}{\eta}+4\right)C_u\sqrt{3}h_L+\rho_\tau+h_t\leq 2\left(\frac{1}{\eta}+6\right)C_u\sqrt{3}h_L.$$

The number of those panels t is bounded by the numbers of cubes $q \in \mathcal{Q}_L$ touching $\mathcal{B}(\tau)$. Since $|\mathcal{B}(\tau)| = O(h_L^3)$ and $|q| = h_L^3$, this number is bounded independent of τ and ℓ .

4.3 Verifying the approximation property of the expansion system

In this subsection, we will prove that the expansion system defined in Definition 32 satisfies Assumption 20 with $m(\ell)$ as in (60). In order to reduce the technicalities in the proofs below we impose a weak assumption (Assumption 58) on the sizes of the sons of a cluster.

Definition 57 Let $c \in T(i)$ and $\tilde{c} \in T(j)$ with j > i and $\tilde{c} \subset c$. The chain

$$\mathcal{K}_{\tilde{c},c} = (c_j, c_{j-1}, c_{j-2}, \dots, c_i)$$

is given by the recursion:

$$c_j = \tilde{c},$$

 $c_{k-1} : \sigma(c_{k-1}) \ni c_k, \qquad k = j, j - 1, \dots, i + 1.$

Assumption 58 There exist positive constants $c_{12}, \bar{\rho} < 1$ so that, for all clusters $c \in T$ and all sons $\tilde{c} \in \sigma(c)$, either $\tilde{c} = c$ or the ratio of the cluster radii satisfies:

$$c_{12} \le \rho_{\tilde{c}}/\rho_c \le \bar{\rho}. \tag{67}$$

For all clusters $c \in T$ and all panels $\tilde{c} \in \mathcal{G}$ with $\tilde{c} \subset c$, the number of repeated clusters in the chain $\mathcal{K}_{\tilde{c},c}$ is bounded by:

$$\sup_{c \in T} \sup_{\substack{\tilde{c} \in \mathcal{G} \\ \tilde{c} \subset c}} n_{\tilde{c},c} \le \overline{n} \tag{68}$$

with

$$n_{\tilde{c},c} := \sharp \left\{ \check{c} \in \mathcal{K}_{\tilde{c},c} \mid \sharp \sigma \left(\check{c} \right) = 1 \right\}. \tag{69}$$

Definition 59 Let $\omega \subset \mathbb{R}^d$ with centre M_{ω} . The Taylor operator $T_{\omega}^{(m)}$ is given formally by

$$T_{\omega}^{(m)}[f](x) = \sum_{|\nu| < m} \gamma_{\nu,\omega}[f] \check{\Phi}_{\omega}^{(\nu)}(x)$$

with

$$\gamma_{\nu,\omega}\left[f\right] = \frac{1}{\nu!} f^{(\nu)}\left(M_{\omega}\right)$$

and

$$\check{\Phi}_{\omega}^{(\nu)}(x) = (x - M_{\omega})^{\nu}. \tag{70}$$

The auxiliary functions $\overrightarrow{\Psi}_{\omega}^{(\nu)}$ are defined by

$$\overrightarrow{\check{\Psi}}_{\omega}^{(\nu)}(y) := \check{\Phi}_{\omega}^{(\nu)}(y) n(y).$$

The expansion functions $\Phi_c^{(\nu)}$ and $\overline{\Psi}_c^{(\nu)}$ (cf. Definition 32) can be regarded as approximations to the functions $\check{\Phi}_{\omega}^{(\nu)}$ and $\dot{\overline{\Psi}}_{\omega}^{(\nu)}$. The precision is concerned in Lemma 61. The normal derivatives of the Taylor polynomials are denoted by

$$\check{N}_{c}^{(\nu)} := \sum_{i=1}^{3} n_{i}(y) \,\check{\Phi}_{c}^{(\nu+e_{i})}(y) = \langle n, y - M_{c} \rangle \,\check{\Phi}_{c}^{(\nu)}$$
(71)

while an analogous quantity for the true expansion system is defined by

$$N_c^{(\nu)} := \sum_{i=1}^3 n_i(y) \, \Phi_c^{(\nu+e_i)}(y) \,. \tag{72}$$

It remains to define the constants a, b for the function $m(\ell) = a(L - \ell) + b$ determining the degree of approximation on a block.

Definition 60 Let Assumption 20 be satisfied. For $0 \le \ell \le L$, the function $m(\ell)$ determining the variable order of approximation is given by

$$m(\ell) = a(L - \ell) + b, \tag{73}$$

with $a, b \in \mathbb{N}_0$ chosen so that

$$a > 1$$
 and $2C_2^a =: C_8 < 1$ (74)

(cf. Remark 65) and

$$b \ge \max \left\{ \frac{\left| \log \frac{1-\bar{\rho}}{2\bar{\rho}} \right|}{\left| \log \bar{\rho} \right|}, 1 + \frac{a \log \lambda_4}{\left| \log \frac{1+\bar{\rho}}{2} \right|}, 2 \left(a \frac{\log \lambda_4}{\log 2} - 1 \right), \frac{\log 2}{\left| \log \bar{\rho} \right|}, \frac{\log \frac{\lambda_4^4 + C_\Gamma - 1}{2(1 - \lambda_4^{-a})}}{\log \frac{4}{3}} \right\}$$
 (75)

with $\lambda_4 > 8$.

Note that the conditions on a and b stem from the proof of the approximation property which we expect are by far too restrictive. In a forthcoming paper, the results of numerical experiments will be presented dealing with the optimal choice of $a, b, \bar{\eta}$ for practical problems.

Lemma 61 Let Assumptions 20, 42, 58, 50, 51, and 53 be satisfied. For all $\lambda_4 \geq c_{12}^{-1}$ (cf. (67)),

$$\omega > \max\left\{\frac{(a+3)^{a+1}}{2(a-1)!}, \frac{2}{1-\bar{\rho}}, e\lambda_4\right\}, \qquad \omega_2 > C_7 \left(1+\omega\right) \max\left\{\sqrt{2C_{\Gamma}\frac{(a+3)^{a+2}}{(a-1)!}}, e\lambda_4\right\}$$
 (76)

and, for all $0 \le \ell \le L$ and all $c \in T(\ell)$, the estimates

$$\left\| \check{\Phi}_{c}^{(\nu)} - \Phi_{c}^{(\nu)} \right\|_{L^{\infty}(c)} \leq \lambda_{4}^{a\bar{n} - m_{\ell}} \left(\omega \rho_{\ell} \right)^{|\nu|} \qquad \forall \nu : |\nu| \leq m \, (\ell) \,,$$

$$\left\| \check{N}_{c}^{(\nu)} - N_{c}^{(\nu)} \right\|_{L^{\infty}(c)} \leq \frac{C_{\Gamma} \lambda_{4}^{a\bar{n}}}{1 - \lambda_{4}^{-a}} \lambda_{4}^{-m_{\ell}} \left(\omega_{2} 2^{-\ell} \right)^{|\nu| + 2} \quad \forall \nu : |\nu| \leq m \, (\ell) - 1$$
(77)

hold with \bar{n} as in (68).

Since the proof of this Lemma is rather technical it is postponed to the Appendix. The approximation of the kernel function on a block $\mathbf{c} = (c_1, c_2) \in P^{(2)}(\ell)$ is given by

$$k(x,y) \approx k_{\mathbf{c}}^{(m)}(x,y) := \sum_{(\nu,\mu)\in\mathbf{I}_m} \overrightarrow{\kappa}_{\nu,\mu}^{(m)}(\mathbf{c}) \Phi_{c_1}^{(\nu)}(x) \overrightarrow{\Psi}_{c_2}^{(\mu)}(y)$$
 (78)

with $m = m(\ell)$ and $\overrightarrow{\kappa}_{\nu,\mu}^{(m)}$ as in (22) and $\Phi_{c_1}^{(\nu)}$, $\overrightarrow{\Psi}_{c_2}^{(\mu)}$ as in Definition 32. The error analysis consists of a consistency and stability part.

For the error analysis, it is preferably to write the Taylor approximation according to (22) in a different form (with n = n(y))⁶

$$\check{k}_{\mathbf{c}}^{(m)}(x,y) = \sum_{|\nu|+|\mu| \le m-1} \left(\sum_{i=1}^{3} n_{i} \check{\Phi}_{c_{1}}^{(\nu+e_{i})}(x) \right) \check{\Phi}_{c_{2}}^{(\mu)}(y) \, \kappa_{\nu,\mu}^{(m)}(\mathbf{c})$$

$$- \sum_{|\nu|+|\mu| \le m-1} \check{\Phi}_{c_{1}}^{(\nu)}(x) \left(\sum_{i=1}^{3} n_{i} \check{\Phi}_{c_{2}}^{(\mu+e_{i})}(y) \right) \kappa_{\nu,\mu}^{(m)}(\mathbf{c})$$

$$+ \langle n, z_{\mathbf{c}} \rangle \sum_{|\nu|+|\mu| \le m-1} \check{\Phi}_{c_{2}}^{(\mu)}(y) \, \check{\Phi}_{c_{1}}^{(\nu)}(x) \, \kappa_{\nu,\mu}^{(m)}(\mathbf{c})$$

$$= : \sum_{s \in \{I,II,III\}} \check{k}_{\mathbf{c}}^{s,(m)}(x,y)$$
(80)

with

$$\kappa_{\nu,\mu}^{(m)}(\mathbf{c}) := \frac{1}{\nu!\mu!} (-1)^{|\mu|} k_3^{(\nu+\mu)}(z_{\mathbf{c}})$$
(81)

and Φ , Ψ as in Definition 59.

Proposition 62 The approximation $k_c^{(m)}$ can be written in the form (79) by replacing the Taylor polynomials $\check{\Phi}_c^{(\nu)}$ by the hierarchical approximations $\Phi_c^{(\nu)}$.

Proof. By definition, $k_{\mathbf{c}}^{(m)}$ has the representation

$$k_{\mathbf{c}}^{(m)}(x,y) := \sum_{i=1}^{3} \sum_{|\nu|+|\mu| \le m} \Phi_{c_{2}}^{(\mu)}(y) \Phi_{c_{1}}^{(\nu)}(x) n_{i} \nu_{i} \frac{(-1)^{|\mu|}}{\mu! \nu!} k_{3}^{(\nu+\mu-e_{i})}(z_{\mathbf{c}})$$

$$+ \sum_{i=1}^{3} \sum_{|\nu|+|\mu| \le m} \Phi_{c_{2}}^{(\mu)}(y) \Phi_{c_{1}}^{(\nu)}(x) n_{i} \mu_{i} \frac{(-1)^{|\mu|}}{\mu! \nu!} k_{3}^{(\nu+\mu-e_{i})}(z_{\mathbf{c}})$$

$$+ \langle n, z_{\mathbf{c}} \rangle \sum_{|\nu|+|\mu| < m} \Phi_{c_{2}}^{(\mu)}(y) \Phi_{c_{1}}^{(\nu)}(x) \frac{(-1)^{|\mu|}}{\mu! \nu!} k_{3}^{(\nu+\mu)}(z_{\mathbf{c}})$$

$$= : \sum_{s \in \{I, II, III\}} k_{\mathbf{c}}^{s,(m)}(x, y). \tag{82}$$

This expansion is derived by re-substituting $z - z_c = x - M_{c_1} - (y - M_{c_2})$ in (21), writing $\langle n, z \rangle = \langle n, x - M_{c_1} \rangle - \langle n, y - M_{c_2} \rangle + \langle n, z_c \rangle$, and re-organizing the sums and products.

Performing the same index manipulations as for the derivation of (22) yields the assertion. ■

For the estimate of the approximation error, we employ the splitting:

$$e_{\mathbf{c}}(x,y) := k(x,y) - k_{\mathbf{c}}^{(m)}(x,y) = \underbrace{k(x,y) - \check{k}_{\mathbf{c}}^{(m)}(x,y)}_{=:e_{\mathbf{c}}^{I}(x,y)} + \underbrace{\check{k}_{\mathbf{c}}^{(m)}(x,y) - k_{\mathbf{c}}^{(m)}(x,y)}_{=:e_{\mathbf{c}}^{II}(x,y)}.$$
(83)

The estimate of $e_{\mathbf{c}}^{I}(x,y)$ directly follows from Lemma 21 and we proceed with considering $e_{\mathbf{c}}^{II}(x,y)$. By employing (79), (80), and (82) the difference $\check{k}_{\mathbf{c}}^{(m)} - k_{\mathbf{c}}^{(m)}$ can be split into three parts:

$$e_{\mathbf{c}}^{II} = \check{k}_{\mathbf{c}}^{(m)} - k_{\mathbf{c}}^{(m)} = \sum_{s \in \{I,II,III\}} \check{k}_{\mathbf{c}}^{s,(m)} - k_{\mathbf{c}}^{s,(m)} =: \sum_{s \in \{III,IV,V\}} e_{\mathbf{c}}^{s}.$$
(84)

We work out the details only for the case $e_{\mathbf{c}}^{III}$ while the estimate of the errors $e_{\mathbf{c}}^{IV,V}$ is just a repetition of the arguments:

$$e_{\mathbf{c}}^{III}(x,y) = \sum_{|\nu|+|\mu|< m} \left(\check{\Phi}_{c_{1}}^{(\nu)}(x) - \Phi_{c_{1}}^{(\nu)}(x)\right) \left(\sum_{i=1}^{3} n_{i} \check{\Phi}_{c_{2}}^{\mu+e_{i}}(y)\right) \kappa_{\nu,\mu}^{(m)}(\mathbf{c}) + \sum_{|\nu|+|\mu|< m} \Phi_{c_{1}}^{(\nu)}(x) \left(\sum_{i=1}^{3} n_{i} \left(\check{\Phi}_{c_{2}}^{\mu+e_{i}}(y) - \Phi_{c_{2}}^{\mu+e_{i}}\right)\right) \kappa_{\nu,\mu}^{(m)}(\mathbf{c})$$

$$= : e_{\mathbf{c}}^{VI}(x,y) + e_{\mathbf{c}}^{VII}(x,y).$$
(85)

In order to estimate $e_{\mathbf{c}}^{VI}, e_{\mathbf{c}}^{VII}$ we need an auxiliary result estimating the size of $\kappa_{\nu,\mu}^{(m)}$.

Lemma 63 Let $\mathbf{c} = (c_1, c_2)$ be η -admissible. Then,

$$\kappa_{\nu,\mu}^{(m)}(\mathbf{c}) = 27 \frac{(\nu + \mu)!}{\nu! \mu!} \left(\frac{4}{\operatorname{dist}(c_1, c_2)} \right)^{|\nu + \mu| + 3}.$$

Proof. We start with estimating the derivatives of the function $k_3: d_{\mathbf{c}} \to \mathbb{R}$ as in (20). Note that all $z \in d_{\mathbf{c}}$ satisfy $||z|| \geq \operatorname{dist}(c_1, c_2)$. For any $w \in \mathbb{C}^3$ with $||w||_{\infty} \leq ||z_{\mathbf{c}}|| / (2\sqrt{3})$ (with $z_{\mathbf{c}} = M_{c_1} - M_{c_2}$), we have

$$||z_{\mathbf{c}} + w|| \ge ||z_{\mathbf{c}}|| - ||w|| \ge ||z_{c}|| - \sqrt{3} ||w||_{\infty} \ge ||z_{\mathbf{c}}|| / 2 \ge \frac{1}{2} \operatorname{dist}(c_{1}, c_{2}).$$

Hence, the function

$$g_3(w) := ||z_{\mathbf{c}} + w||^{-3}$$

is holomorphic with respect to each component in $B_{r_1}(0)$, i.e., in the ball in complex plane centred at the origin with radius $r_1 := ||z_{\mathbf{c}}|| / (2\sqrt{3})$. Applying Cauchy's integral formula in each component results in

$$\frac{1}{\mu!}g_3^{(\mu)}(w) = \frac{1}{(2\pi i)^3} \oint_{|v_1|=r} \oint_{|v_2|=r} \oint_{|v_3|=r} \frac{g_3(v)}{(v-w)^{\mu+1}} dv$$

with $\mathbf{1} = (1, 1, 1)^{\mathsf{T}}$ and $r = 3 \|z_{\mathbf{c}}\| / 4$. The function g_3 can be estimated by

$$|g_3(v)| \le \left(\frac{1}{4} \|z_{\mathbf{c}}\|\right)^{-3}.$$

The denominator satisfies

$$|(v-w)^{\mu+1}| \ge \prod_{i=1}^{3} (|v_i| - |w_i|)^{\mu_i+1} \ge \prod_{i=1}^{3} \left(\frac{1}{4} ||z_{\mathbf{c}}||\right)^{\mu_i+1} = \left(\frac{1}{4} ||z_{\mathbf{c}}||\right)^{|\mu|+3}$$

and the length of a single integral path $2\pi r = 3\pi ||z_{\mathbf{c}}||/2$. Hence,

$$\left| \frac{1}{\mu!} g_3^{(\mu)}(w) \right| \le \frac{1}{8\pi^3} \left(3\pi \|z_{\mathbf{c}}\| / 2 \right)^3 \left(\frac{1}{4} \|z_{\mathbf{c}}\| \right)^{-3} \frac{1}{\left(\frac{1}{4} \|z_{\mathbf{c}}\| \right)^{|\mu|+3}} = 27 \left(\frac{4}{\|z_{\mathbf{c}}\|} \right)^{|\mu|+3}.$$

The connection between g_3 and k_3 is given by $k_3^{(\mu)}(z_c) = g_3^{(\mu)}(0)$ and, hence,

$$\left| k_3^{(\mu)}(z_{\mathbf{c}}) \right| = \left| g_3^{(\mu)}(0) \right| \le 27\mu! \left(\frac{4}{\|z_{\mathbf{c}}\|} \right)^{|\mu|+3}.$$

In view of (81), we obtain the assertion:

$$\left|\kappa_{\nu,\mu}^{(m)}\left(\mathbf{c}\right)\right| = 27 \frac{(\nu+\mu)!}{\nu!\mu!} \left(\frac{4}{\|z_{\mathbf{c}}\|}\right)^{|\nu+\mu|+3}.$$

Theorem 64 Let \mathbf{I}_m , ι_m^I , ι_m^{II} , and the expansion systems $\Phi_c^{(\nu)}$, $\Psi_c^{(\nu)}$ be chosen as in Definition 32 and the distribution of the expansion order as in Definition 60. Let the Assumptions of Lemma 61 be satisfied. Then, there exists $\overline{\eta}$ depending only on C_6 , C_7 , λ_3 , a, b, c_{12} , $\overline{\rho}$ so that the expansion (78) satisfies Assumption 20.

Proof. In view of (83) along with Lemma 21 we may restrict to the estimate of $e_{\mathbf{c}}^{II}$. As before, we work out the proof only for the partial error $e_{\mathbf{c}}^{III}$ in (84) while the estimate of $e_{\mathbf{c}}^{IV,V}$ is just a repetition of the arguments. Hence, it is sufficient to estimate the errors $e_{\mathbf{c}}^{VI}$ and $e_{\mathbf{c}}^{VII}$ (see (85)). Using Lemma 61 and 63 along with

$$\left| \sum_{i=1}^{3} n_{i} \check{\Phi}_{c}^{\mu+e_{i}} (y) \right| = \left| \left\langle n (y), y - M_{c} \right\rangle (y - M_{c})^{\mu} \right| \leq C_{\Gamma} \rho_{\ell}^{|\mu|+2}, \quad \forall x \in c \in T (\ell),$$

we obtain (putting $m = m(\ell)$):

$$\begin{aligned} \left| e_{\mathbf{c}}^{VI} \left(x, y \right) \right| & \leq 27 \sum_{|\nu| + |\mu| < m_{\ell}} \lambda_{4}^{a\bar{n} - m_{\ell}} \left(\omega \rho_{\ell} \right)^{|\nu|} \left(C_{\Gamma} \rho_{\ell}^{|\mu| + 2} \right) \frac{(\nu + \mu)!}{\nu! \mu!} \left(\frac{4}{\operatorname{dist} \left(c_{1}, c_{2} \right)} \right)^{|\nu + \mu| + 3} \\ & \leq \tilde{C} \operatorname{dist}^{-1} \left(c_{1}, c_{2} \right) \lambda_{4}^{-m_{\ell}} \sum_{|\nu| + |\mu| < m_{\ell}} \binom{\nu + \mu}{\nu} \left(\frac{4\omega \rho_{\ell}}{\operatorname{dist} \left(c_{1}, c_{2} \right)} \right)^{|\nu + \mu| + 2} \end{aligned}$$

with $\tilde{C} = 4 \times 27 C_{\Gamma} \lambda_4^{a\bar{n}}$. By using $\rho_{\ell}/\operatorname{dist}(c_1, c_2) \leq \eta$ and choosing $\bar{\eta} < (4\omega)^{-1}$ we get

$$\sum_{|\nu|+|\mu|< m_{\ell}} {\nu + \mu \choose \nu} \left(\frac{4\omega \rho_{\ell}}{\operatorname{dist}(c_{1}, c_{2})} \right)^{|\nu+\mu|+2} \leq \sum_{|\nu|+|\mu|< m_{\ell}} {\nu + \mu \choose \nu} \leq 2^{3m_{\ell}} = 8^{m_{\ell}}.$$

Thus,

$$\left| e_{\mathbf{c}}^{VI}(x,y) \right| \le \tilde{C} \operatorname{dist}^{-1}(c_1, c_2) \lambda_4^{-m_{\ell}} 8^{m_{\ell}}.$$
 (86)

By choosing $\lambda_4 > 8$, we have proven an estimate of the form (11).

It remains to estimate $e_{\mathbf{c}}^{VII}$. The norm of the expansion functions $\Phi_{c_1}^{(\nu)}$ can be estimated by

$$\begin{split} \left\| \Phi_{c_{1}}^{(\nu)} \right\|_{L^{\infty}(c_{1})} &= \left\| \check{\Phi}_{c_{1}}^{(\nu)} \right\|_{L^{\infty}(c_{1})} + \left\| \Phi_{c_{1}}^{(\nu)} - \check{\Phi}_{c_{1}}^{(\nu)} \right\|_{L^{\infty}(c_{1})} \\ &\leq \rho_{\ell}^{|\nu|} + \lambda_{4}^{a\bar{n} - m_{\ell}} \left(\omega \rho_{\ell} \right)^{|\nu|} \leq \rho_{\ell}^{|\nu|} \left(1 + \lambda_{4}^{a\bar{n} - m_{\ell}} \omega^{|\nu|} \right) \\ &\leq \rho_{\ell}^{|\nu|} \left(1 + \lambda_{4}^{a\bar{n}} \omega \right)^{|\nu|} =: \left(\tilde{\omega} \rho_{\ell} \right)^{|\nu|} \end{split} \tag{87}$$

with suitable $\tilde{\omega}$. Hence, by using (85) in combination with (87), (77), Lemma 63, and Assumption 42 we get

$$\begin{aligned} \left| e_{\mathbf{c}}^{VII} \left(x, y \right) \right| & \leq \frac{C_{\Gamma} \lambda_{4}^{a\bar{n}}}{1 - \lambda_{4}^{-a}} \sum_{|\nu| + |\mu| < m} \left(\tilde{\omega} \rho_{\ell} \right)^{|\nu|} \lambda_{4}^{-m_{\ell}} \left(\omega_{2} 2^{-\ell} \right)^{|\mu| + 2} 27 \frac{(\nu + \mu)!}{\nu! \mu!} \left(\frac{4}{\operatorname{dist} \left(c_{1}, c_{2} \right)} \right)^{|\nu + \mu| + 3} \\ & \leq \check{C} \lambda_{4}^{-m_{\ell}} \operatorname{dist}^{-1} \left(c_{1}, c_{2} \right) \sum_{|\nu| + |\mu| < m} \frac{(\nu + \mu)!}{\nu! \mu!} \left(\frac{4M_{\omega} 2^{-\ell}}{\operatorname{dist} \left(c_{1}, c_{2} \right)} \right)^{|\nu + \mu| + 2} \end{aligned}$$

where $M_{\omega} = \max\{C_7\tilde{\omega}, \omega_2\}$. Assumption 42 implies $2^{-\ell} \leq C_7\rho_{\ell}$ and, hence, the rest of the estimate is just a repetition of the arguments used for proving (86): For sufficiently small $\bar{\eta}$, an estimate of the form

$$\left| e_{\mathbf{c}}^{III}\left(x,y \right) \right| \leq \tilde{C} C_{2,III}^{m_{\ell}} \operatorname{dist}^{-1}\left(c_{1},c_{2} \right)$$

holds with $C_{2,III} < 1$. Similarly, the error contributions $e_{\mathbf{c}}^{IV}$ and $e_{\mathbf{c}}^{V}$ (cf. (84)) can be estimated.

Remark 65 For the approximation $k_{\mathbf{c}}^{(m)}(x,y)$ as in (78), the constant C_2 in Assumption 20 is **independent** of a in (56) (cf. (86)). Hence, the constant a could be chosen so that

$$\lambda_2 C_2^a =: C_8 < 1.$$

5 Complexity analysis

In this section, we will prove that, for quasi-uniform and shape regulars meshes, the storage amount and complexity of the variable order panel clustering method depend only linearly on the number of unknowns without any logarithmic terms. The key role in these proofs is played by sharp estimates on the number of blocks contained in the farfield levels $F(\ell)$ and in the nearfield N. Let n denote the number of panels, i.e., $n = \sharp \mathcal{G} = \dim S^{-1,0}$.

Lemma 66 Let Assumption 50 be satisfied. There exist positive constants C_{13} , C_{14} so that, for all $0 \le \ell \le L$, the number of nearfield and farfield blocks is bounded by

$$\sharp F(\ell) \leq C_{13}4^{\ell}, \tag{88}$$

$$\sharp N \leq C_{14}n. \tag{89}$$

Proof. First, we prove (88). By construction (cf. procedure **build_cluster_tree**) the cluster tree T is balanced implying $F(\ell) \subset T(\ell) \times T(\ell)$. In view of Lemma 55 and Lemma 56 it is sufficient to proof that there exists a constant C_{15} so that, for all $0 \le \ell \le L$,

$$\sharp T\left(\ell\right) \leq C_{15}4^{\ell}.$$

All cluster centres M_{τ} of panels $\tau \in \mathcal{G}$ are contained in an h-neighbourhood $U_h(\Gamma)$ of Γ which was already introduced in Notation 49. The number of clusters contained in $T(\ell)$ is bounded from above by the number of cubes $q \in \mathcal{Q}_{\ell}$ satisfying

$$U_h\left(\Gamma\right) \cap q \neq \emptyset. \tag{90}$$

All cubes with this property are contained in $U_{h+d}(\Gamma)$ with $d = \sqrt{3} \times 2^{-\ell}$. Due to the quasi-uniformity of the grid, there exists $C < \infty$ so that $h + d \leq C2^{-\ell}$. Hence, all cubes with property (90) are contained in $U_{C2^{-\ell}}(\Gamma)$. Due to Assumption 50 we have

$$|U_{C2^{-\ell}}| \le C_{\Gamma} C 2^{-\ell}.$$

The volume of q is $2^{-3\ell}$ and, hence, the number of such cubes are bounded from above by

$$\frac{|U_{C2^{-\ell}}|}{2^{-3\ell}} \le C_{\Gamma}C4^{\ell}.$$

It remains to prove (89). The estimate follows directly from $\sharp \mathcal{G} = n$ and Lemma 56. \blacksquare

The depth of the cluster tree is concerned in the next lemma.

Lemma 67 Let Assumption 50, 51, and 53 be satisfied and the cluster tree constructed by the procedure **build_cluster_tree**. Then,

$$4^L \le \frac{12C_u^2}{|\Gamma|} n.$$

Proof. Condition (35) implies $\sqrt{3}h_L \geq \underline{\rho}$. Taking into account Definition 36 and 37 along with

$$|\Gamma| = \sum_{\tau \in \mathcal{G}} |\tau| \le nh^2$$

we obtain

$$4^{L} \le 3\underline{\rho}^{-2} \le \frac{12C_u^2}{h^2} \le \frac{12C_u^2}{|\Gamma|}n.$$

The following lemma estimates the amount of work per tree and farfield level. It has auxiliary character and will be used in the complexity estimates below.

Lemma 68 Let $a, b, s \geq 0$. Then,

$$\sum_{\ell=0}^{L} (a (L - \ell) + b)^{s} 4^{\ell} \le 2 \left(\frac{s (a + b)}{\ln 2} \right)^{s} 4^{L}.$$

Proof. Simple analysis yields:

$$\sum_{\ell=0}^{L} (a(L-\ell)+b)^{s} 4^{\ell} \leq (a+b)^{s} \sum_{\ell=0}^{L} (L-\ell+1)^{s} 4^{\ell} = (a+b)^{s} 4^{L} \sum_{\ell=0}^{L} (\ell+1)^{s} 4^{-\ell}$$

$$\leq (a+b)^{s} 4^{L} \left(\frac{s}{\ln 2}\right)^{s} \sum_{\ell=0}^{L} 2^{\ell} 4^{-\ell} = 2 \left(\frac{s(a+b)}{\ln 2}\right)^{s} 4^{L}.$$

In the sequel, we will estimate the number of operations in the single steps of the variable order panel clustering algorithm.

(a) Procedure **build_cluster_tree**.

Clearly, the complexity of the procedure is proportional to the number of elements in the cluster tree:

$$\sharp T = \sum_{\ell=0}^{L} 4^{\ell} \le \frac{4}{3} 4^{L} \le \frac{16C_u^2}{|\Gamma|} n.$$

(b) Computation of the expansion coefficients.

In [8], [15], [9], algorithms are presented where the computation of

$$\overrightarrow{\kappa}_{\nu,\mu}^{m}(\mathbf{c}), \quad \forall \nu, \mu \in \mathbf{I}_{m}$$

can be performed in $O(m^7)$ operation. Hence, the computation for all coefficients and all farfield blocks costs (cf. (88) and Lemma 68)

$$\sum_{\ell=0}^{L} m^{7}(\ell) \times \sharp F(\ell) \le C_{13} \sum_{\ell=0}^{L} (a(L-\ell) + b)^{7} 4^{\ell} \le Cn$$
 (91)

where C only depends on a, b, C_{13}, C_u , and $|\Gamma|$.

(c) Computation of the farfield coefficients.

The computation of all farfield coefficients $J^I_{\tau,\nu}$ and $J^{II}_{\tau,\mu}$ for the panels $\tau \in \mathcal{G}$ and $\nu \in \iota^I_{m(L)}$, $\mu \in \iota^{II}_{m(L)}$ is proportionally to n due m(L) = b.

The procedure **build_cluster_tree** implies that the number of sons of a cluster is bounded from above by 64. Thus, the evaluation of the recursion (49) costs O(1) operation per farfield coefficients. Similar computations as in (91) yield that the number of operations is proportional to n.

- (d) Computation of the recursion coefficients $\gamma_{\nu,\tilde{\nu},\tilde{c}}$ in (48). From (45), it follows directly, that the amount of computational work per coefficients is O(1) while the total number of coefficients is bounded by O(n).
 - (e) Evaluation of a matrix vector multiplication.

By similar considerations, one obtains that the evaluation of a matrix vector multiplication, i.e., Algorithm 35, costs O(n) operations.

(f) Storage amount.

By using the same technique as for the computational complexity one can prove that the amount of memory for storing the quantities \mathcal{G} , T, F, $\kappa_{\nu,\mu}^{m}(\mathbf{c})$, $J_{c,\nu}^{I}$, $J_{c,\mu}^{II}$, and $\gamma_{\nu,\tilde{\nu},\tilde{c}}$ (as in (45)) is proportionally to n.

Theorem 69 Let Assumption 50, 51, and 53 be satisfied and the cluster tree constructed by the procedure **build_cluster_tree**. The variable order panel clustering algorithm has linear complexity with respect to the computing time and the memory consumption.

6 Appendix

In this appendix, we prove Lemma 61 and some auxiliary estimates. We adopt the notation of the proof of Lemma 61.

Proof of Lemma 61:

Let $\tilde{m} = m (\ell + 1)$. We define an intermediate approximation to $\check{\Phi}_c^{(\nu)}$ by restricting the sum in (44) to $\tilde{\nu} \in \iota_{\tilde{c}}$:

$$\tilde{\Phi}_{\tilde{c}}^{(\nu)} := \sum_{\tilde{\nu} \in \iota_{\tilde{c}}} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}, \qquad \forall \tilde{c} \in \sigma (c)$$

with $\gamma_{\nu,\tilde{\nu},\tilde{c}}$ as in (45). On \tilde{c} , the representation

$$\check{\Phi}_{c}^{(\nu)} - \Phi_{c}^{(\nu)} = \check{\Phi}_{c}^{(\nu)} - \tilde{\Phi}_{\tilde{c}}^{(\nu)} + \sum_{\tilde{\nu} \in \iota_{\tilde{c}}} \gamma_{\nu,\tilde{\nu},\tilde{c}} \left(\check{\Phi}_{\tilde{c}}^{(\tilde{\nu})} - \Phi_{\tilde{c}}^{(\tilde{\nu})} \right)$$

⁷Let $c \in T(\ell)$ with reference cube $q = \text{REF}(c) \in \mathcal{Q}_{\ell}$. The possible sons are the pullbacks of all cubes $\tilde{q} \in \mathcal{Q}_{\ell+1}$ with $\overline{\tilde{q}} \cap \overline{q} \neq \emptyset$. The number of those cubes is 64.

holds. Let $\tau \in \mathcal{G}$ so that $\tau \subset \tilde{c} \in \sigma(c)$ and let the chain $\mathcal{K}_{\tau,c}$ be as in Definition 57. For $\ell \leq i \leq L$, define

$$\delta_i^{(\nu)} := \left\| \check{\Phi}_{t_i}^{(\nu)} - \Phi_{t_i}^{(\nu)} \right\|_{L^{\infty}(\tau)}, \qquad \varepsilon_i^{(\nu)} = \left\| \check{\Phi}_{t_i}^{(\nu)} - \tilde{\Phi}_{t_{i+1}}^{(\nu)} \right\|_{L^{\infty}(\tau)}. \tag{92}$$

Then,

$$\delta_i^{(\nu)} \le \varepsilon_i^{(\nu)} + \sum_{\tilde{\nu} \in \iota_{m(i+1)}} \left| \gamma_{\nu,\tilde{\nu},t_{i+1}} \right| \delta_{i+1}^{(\tilde{\nu})}.$$

The cluster radius ρ_{t_i} is abbreviated by ρ_i . In Lemma 70, we prove

$$\delta_i^{(\nu)} \le \lambda_4^{a\bar{n} - m_i} \left(\omega \rho_i\right)^{|\nu|} \tag{93}$$

for some $\lambda_4 > 1$ and sufficiently large ω depending only on $a, \bar{\rho}, \lambda_4$. Since $\tau \in \mathcal{G}$ was chosen arbitrary, we have shown that

$$\left\| \check{\Phi}_{c}^{(\nu)} - \Phi_{c}^{(\nu)} \right\|_{L^{\infty}(c)} \leq \lambda_{4}^{a\bar{n} - m_{i}} \left(\omega \rho_{\ell} \right)^{|\nu|}$$

holds.

We turn to the second estimate in (77) and introduce the intermediate approximation to $\tilde{N}_c^{(\nu)}$ (cf. (71))

$$\tilde{N}_{c}^{(\nu)}(y) := \sum_{i=1}^{3} n_{i}(y) \,\tilde{\Phi}_{c}^{(\nu+e_{i})}(y).$$
 (94)

In Lemma 72, the recursions (for $x \in \tilde{c}$)

$$\tilde{N}_{c}^{(\nu)}(x) = \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| \leq \tilde{m}} \gamma_{\nu,\tilde{\nu},\tilde{c}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}(x) + \sum_{|\tilde{\nu}| \leq \tilde{m} - 1} \gamma_{\nu,\tilde{\nu},\tilde{c}} \check{N}_{\tilde{c}}^{(\tilde{\nu})}(x) \qquad (95)$$

$$N_{c}^{(\nu)}(x) = \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| < \tilde{m}} \gamma_{\nu,\tilde{\nu},\tilde{c}} \Phi_{\tilde{c}}^{\tilde{\nu}}(x) + \sum_{|\tilde{\nu}| < \tilde{m} - 1} \gamma_{\nu,\tilde{\nu},\tilde{c}} N_{\tilde{c}}^{(\tilde{\nu})}(x)$$

are proved. For $\ell \leq i \leq L$, define

$$\theta_i^{(\nu)} := \left\| \check{N}_{t_i}^{(\nu)} - N_{t_i}^{(\nu)} \right\|_{L^{\infty}(\tau)}, \qquad \pi_i^{(\nu)} = \left\| \check{N}_{t_i}^{(\nu)} - \tilde{N}_{t_{i+1}}^{(\nu)} \right\|_{L^{\infty}(\tau)}. \tag{96}$$

Equations (71), (72), and (94) imply that

$$\theta_i^{(\nu)} = 0, \qquad \forall \nu : |\nu| + 1 \le b, \qquad \forall \ell \le i \le L. \tag{97}$$

Hence, it remains to consider the case $|\nu| \geq b$. The error $\theta_i^{(\nu)}$ can be estimated by

$$\theta_{i}^{(\nu)} \leq \pi_{i}^{(\nu)} + \left| \left\langle n, M_{t_{i+1}} - M_{t_{i}} \right\rangle \right| \sum_{|\tilde{\nu}| \leq m_{i+1}} \left| \gamma_{\nu, \tilde{\nu}, \tilde{c}} \right| \delta_{i+1}^{(\tilde{\nu})} + \sum_{|\tilde{\nu}| < m_{i+1}} \left| \gamma_{\nu, \tilde{\nu}, \tilde{c}} \right| \theta_{i+1}^{(\tilde{\nu})}. \tag{98}$$

In Lemma 73, we will prove that

$$\pi_i^{(\nu)} \le \begin{cases} 0, & \forall \nu : |\nu| < m_{i+1} \\ C_i \rho_i^{|\nu|+2} \left(\frac{\rho_{i+1}}{\rho_i}\right)^{m_{i+1}+1} {|\nu| \choose m_{i+1}+1} & \forall \nu : m_{i+1} \le |\nu| < m_i \end{cases}$$
(99)

holds with $C_i = C_{\Gamma} (m_{i+1} + 3)^3$.

In the next step, the second term (98) will be estimated. The smoothness of the surface and Lemma 70 imply

$$\left| \left\langle n, M_{t_{i+1}} - M_{t_{i}} \right\rangle \right| \sum_{|\tilde{\nu}| \leq \tilde{m}} |\gamma_{\nu, \tilde{\nu}, \tilde{c}}| \, \delta_{i+1}^{(\tilde{\nu})} \leq C_{\Gamma} \rho_{i}^{2} \lambda_{4}^{an_{i+1} - m_{i+1}} \rho_{i}^{|\nu|} \sum_{\tilde{\nu} \leq \nu} {\nu \choose \tilde{\nu}} \omega^{|\tilde{\nu}|}$$

$$\leq C_{\Gamma} \lambda_{4}^{an_{i+1} - m_{i+1}} \left(\tilde{\omega} \rho_{i} \right)^{|\nu| + 2} =: f_{i}^{(\nu)}$$

$$(100)$$

with $\tilde{\omega} = (1 + \omega)$. For $|\nu| < m_{i+1}$, estimate (99) implies $V_i^{(\nu)} := \pi_i^{(\nu)} + f_i^{(\nu)} = f_i^{(\nu)}$ and, for $m_{i+1} \leq |\nu| < m_i$, we have

$$\pi_i^{(\nu)} + f_i^{(\nu)} \le 2C_i \lambda_4^{an_{i+1}} \left(\tilde{\omega}\rho_i\right)^{|\nu|+2} \left(\frac{\rho_{i+1}}{\rho_i}\right)^{m_{i+1}} \binom{|\nu|}{m_{i+1}+1} =: V_i^{(\nu)} \tag{101}$$

provided $\lambda_4 \geq c_{12}^{-1}$ (cf. Assumption 58). Together, we have proved that the error $\theta_i^{(\nu)}$ can be estimated by

$$\theta_i^{(\nu)} \le V_i^{(\nu)} + \sum_{|\tilde{\nu}| < m_{i+1}} |\gamma_{\nu,\tilde{\nu},\tilde{c}}| \, \theta_{i+1}^{(\tilde{\nu})}, \qquad \forall \nu : |\nu| < m_i.$$
 (102)

In Lemma 71, we will prove that

$$\theta_i^{(\nu)} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} + S_i^{(\nu)} \quad \text{with } S_i^{(\nu)} = \sum_{k=i}^{L-1} f_k^{(\nu)}$$
 (103)

holds. By using (120) and $\lambda_4^{-a} < 1$ we obtain

$$\theta_i^{(\nu)} \le \lambda_4^{-m_i} \left(\omega_2 2^{-i}\right)^{|\nu|+2} \frac{C_\Gamma \lambda_4^{a\overline{n}}}{1 - \lambda_4^{-a}}.$$

Lemma 70 Let the Assumptions of Lemma 61 be satisfied. Then, the coefficients $\delta_i^{(\nu)}$ defined in (92) can be estimated by

$$\left|\delta_i^{(\nu)}\right| \leq \lambda_4^{an_i - m_i} \left(\omega \rho_i\right)^{|\nu|}$$

with $n_i := n_{\tau,t_i}$ (cf. Definition 58).

Proof. Set $m = m_i$ and $\tilde{m} = m_{i+1}$. Estimates (122) and (123) imply (for $|\nu| > \tilde{m}$):

$$\left| \left(\check{\Phi}_c^{(\nu)} - \tilde{\Phi}_{\tilde{c}}^{(\nu)} \right)(x) \right| \le \tilde{C}_i \binom{|\nu|}{\tilde{m}+1} \rho_i^{|\nu|} \left(\frac{\rho_{i+1}}{\rho_i} \right)^{\tilde{m}+1}$$

with

$$\tilde{C}_i = (\tilde{m} + 3)(\tilde{m} + 2)/2$$
 (104)

resulting in

$$\varepsilon_{i}^{(\nu)} \leq \begin{cases} 0 & \nu \in \iota_{\tilde{m}}, \\ \tilde{C}_{i}\binom{|\nu|}{\tilde{m}+1}\rho_{i}^{|\nu|} \left(\frac{\rho_{i+1}}{\rho_{i}}\right)^{\tilde{m}+1} & \nu \in \iota_{m} \setminus \iota_{\tilde{m}}. \end{cases}$$
(105)

The coefficients $\gamma_{\nu,\tilde{\nu},\tilde{c}}$ can be estimated,

• for $\tilde{c} = c$, by

$$|\gamma_{\nu,\widetilde{\nu},\widetilde{c}}| \le \begin{cases} 1 & \nu = \widetilde{\nu} \\ 0 & \text{otherwise} \end{cases}$$
 (106)

• for $\tilde{c} \in \sigma(c)$ and $\tilde{c} \neq c$, by

$$|\gamma_{\nu,\widetilde{\nu},\widetilde{c}}| \le \begin{cases} \binom{\nu}{\widetilde{\nu}} \rho_i^{|\nu-\widetilde{\nu}|} & \text{if } \widetilde{\nu} \le \nu\\ 0 & \text{otherwise} \end{cases}$$
 (107)

Next, the coefficients $\delta_i^{(\nu)}$ are estimated. Definition 32 implies that the Taylor polynomials $\check{\Phi}_c^{(\nu)}$ coincide with $\Phi_c^{(\nu)}$ up to the order b (cf. Definition 60):

$$\delta_i^{(\nu)} = 0, \qquad \forall \nu \in \iota_{m(L)}, \qquad \forall \ell \le i \le L.$$
 (108)

Recall that $\iota_{m(L)} = \iota_b = \{ \nu \in \mathbb{N}_0^3 : |\nu| \leq b \}$. Hence, we may assume below that $\nu \notin \iota_{m(L)}$, i.e.,

$$|\nu| > b \tag{109}$$

due to (73). The proof for $|\nu| > b$ is based on an induction over $i = L, L - 1, \ldots, \ell$:

 \bullet i=L:

The assertion directly follows from (108).

• Assumption: Assertion holds up to an index i + 1:

$$\delta_k^{(\nu)} \le \lambda_4^{an_k - m_k} \left(\omega \rho_k \right)^{|\nu|}, \qquad \forall \nu \in \iota_{m(k)}, \qquad \forall k = i + 1, i + 2, \dots L$$
 (110)

where $n_k = n_{\tau,t_k}$ denotes the number of repeated clusters in the chain \mathcal{K}_{τ,t_k} (cf. (69)).

• $i+1 \rightarrow i$:

We first consider the case that $\sigma(t_i) = \{t_{i+1}\}$, i.e., $t_i = t_{i+1}$ (cf. Assumption 58). This implies that the number of repeated cluster is increased by one: $n_{\tau,t_{i+1}} + 1 = n_{\tau,t_i}$ (cf. (69)). We write short $n_{i+1} = n_{\tau,t_{i+1}}$ and $n_i = n_{\tau,t_i}$ and note that $n_i \geq 1$ holds. Taking into account (106) the definition of $\delta_i^{(\nu)}$ reduces to

$$\delta_i^{(\nu)} = \begin{cases} \delta_{i+1}^{(\nu)} & \forall \nu \in \iota_{m(i+1)}, \\ \varepsilon_i^{(\nu)} & \forall \nu \in \iota_{m(i)} \backslash \iota_{m(i+1)}. \end{cases}$$
 (111)

For $\nu \in \iota_{m(i+1)}$, we employ (110) and obtain, by using (109):

$$\delta_{i}^{(\nu)} = \delta_{i+1}^{(\nu)} \leq \lambda_{4}^{an_{i+1}-m_{i+1}} \left(\omega \rho_{i+1}\right)^{|\nu|} = \lambda_{4}^{a} \lambda_{4}^{an_{i+1}-m_{i}} \left(\omega \rho_{i}\right)^{|\nu|} \leq \lambda_{4}^{an_{i}-m_{i}} \left(\omega \rho_{i}\right)^{|\nu|}.$$

It remains to consider $\nu \in \iota_{m(i)} \setminus \iota_{m(i+1)}$, which implies

$$m_i - a < |\nu| \le m_i. \tag{112}$$

Simple combinatorial manipulations show that (cf. (105))

$$\varepsilon_{i}^{(\nu)} \leq C_{i} \binom{|\nu|}{m_{i+1} + 1} \rho_{i}^{|\nu|} \leq C_{i} \frac{m_{i}^{a-1}}{(a-1)!} \rho_{i}^{|\nu|} \\
\leq \lambda_{4}^{an_{i} - m_{i}} (\omega \rho_{i})^{|\nu|} \underbrace{C_{i} \frac{m_{i}^{a-1} \lambda_{4}^{m_{i} - an_{i}}}{(a-1)!} \omega^{-|\nu|}}_{=:\phi}.$$
(113)

It remains to prove that ϕ is bounded by 1, for sufficiently large ω . Estimate (112) and (104) along with $n_i \geq 1$ imply

$$\phi \le C_i \frac{m_i^{a-1} \lambda_4^{m_i - a}}{(a-1)!} \omega^{-(m_i - a + 1)} \le \frac{1}{2\omega (a-1)!} (m_i + 3)^{a+1} \left(\frac{\lambda_4}{\omega}\right)^{m_i - a}.$$

Simple analysis yields (with $\lambda_4/\omega < 1/e$ and $\omega \ge \frac{(a+3)^{a+1}}{2(a-1)!}$)

$$\phi \le \frac{1}{\omega} \frac{(a+3)^{a+1}}{2(a-1)!} \le 1. \tag{114}$$

It remains to discuss the case $t_i \neq t_{i+1}$ implying $\rho_{i+1}/\rho_i \leq \bar{\rho} < 1$ and $n_i = n_{i+1}$. The coefficients $\delta_i^{(\nu)}$ can be estimated by

$$\delta_{i}^{(\nu)} \leq \begin{cases}
\sum_{\tilde{\nu} \in \iota_{m(i+1)} \atop \tilde{\nu} \leq \nu} {\binom{\nu}{\tilde{\nu}} \rho_{i}^{|\nu-\tilde{\nu}|} \delta_{i+1}^{(\tilde{\nu})}} & \forall \nu \in \iota_{m(i+1)}, \\
C_{i} {\binom{|\nu|}{m_{i+1}+1}} \rho_{i}^{|\nu|} + \sum_{\tilde{\nu} \in \iota_{m(i+1)} \atop \tilde{\nu} \leq \nu} {\binom{\nu}{\tilde{\nu}} \rho_{i}^{|\nu-\tilde{\nu}|} \delta_{i+1}^{(\tilde{\nu})}} & \forall \nu \in \iota_{m(i)} \setminus \iota_{m(i+1)}.
\end{cases} (115)$$

Using the assumption (110) we obtain for the sum in (115) the estimate:

$$\sum_{\tilde{\nu}\in\iota_{m(i+1)}} \binom{\nu}{\tilde{\nu}} \rho_{i}^{|\nu-\tilde{\nu}|} \delta_{i+1}^{(\tilde{\nu})} \leq \sum_{\tilde{\nu}\leq\nu} \binom{\nu}{\tilde{\nu}} \rho_{i}^{|\nu-\tilde{\nu}|} \lambda_{4}^{an_{i+1}-m_{i+1}} (\omega \rho_{i+1})^{|\tilde{\nu}|} \tag{116}$$

$$\leq \left(\lambda_{4}^{n_{i}a-m_{i}} (\omega \rho_{i})^{|\nu|}\right) \lambda_{4}^{m_{i}-m_{i+1}} \omega^{-|\nu|} \sum_{\tilde{\nu}\leq\nu} \binom{\nu}{\tilde{\nu}} \left(\frac{\omega \rho_{i+1}}{\rho_{i}}\right)^{|\tilde{\nu}|}$$

$$= \left(\lambda_{4}^{n_{i}a-m_{i}} (\omega \rho_{i})^{|\nu|}\right) \underbrace{\lambda_{4}^{a} \left(\frac{1}{\omega} + \frac{\rho_{i+1}}{\rho_{i}}\right)^{|\nu|}}_{=:\psi}.$$

The quantity ψ can be estimated by using Assumption 58:

$$\psi \le \lambda_4^a \left(\frac{1}{\omega} + \bar{\rho}\right)^{|\nu|}.$$

Choosing $\omega \geq 2/(1-\bar{\rho})$ yields

$$\frac{1}{\omega} + \bar{\rho} \le \frac{1 + \bar{\rho}}{2} < 1.$$

Taking into account (109) and choosing $b \ge 1 + a \ln \lambda_4 / \left| \ln \frac{1 + \bar{\rho}}{2} \right|$ results in

$$\psi \le \lambda_4^a \left(\frac{1+\bar{\rho}}{2}\right)^b \le \frac{1+\bar{\rho}}{2} \le 1.$$

Similar as in (113) along with $\rho_{i+1}/\rho_i \leq \bar{\rho}$ and $\omega \geq \frac{(a+3)^{a+1}}{2(a-1)!}$, the quantity $\varepsilon_i^{(\nu)}$ can be estimated by

$$\varepsilon_{i}^{(\nu)} \leq \lambda_{4}^{an_{i}-m_{i}} (\omega \rho_{i})^{|\nu|} \bar{\rho}^{m_{i+1}+1} \frac{1}{\omega} \frac{(a+3)^{a+1}}{2(a-1)!} < \lambda_{4}^{an_{i}-m_{i}} (\omega \rho_{i})^{|\nu|} \bar{\rho}^{b+1}.$$

Choosing $b \ge \left|\log \frac{1-\bar{\rho}}{2\bar{\rho}}\right|/\left|\log \bar{\rho}\right|$ results in

$$\varepsilon_i^{(\nu)} + \lambda_4^{n_i a - m_i} \left(\omega \rho_i \right)^{|\nu|} \psi \le \lambda_4^{a n_i - m_i} \left(\omega \rho_i \right)^{|\nu|}.$$

Altogether we have proved that

$$\delta_i^{(\nu)} \le \lambda_4^{an_i - m_i} \left(\omega \rho_i \right)^{|\nu|}.$$

The analogous estimate for the error $\theta_i^{(\nu)}$ is proved in Lemma 71.

Lemma 71 Let the assumptions of Lemma 61 be satisfied. Then, the coefficients $\theta_i^{(\nu)}$ defined in (96) can be estimated by

$$\left|\theta_i^{(\nu)}\right| \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} + S_i^{(\nu)}$$

with $n_i := n_{\tau,t_i}$ (cf. Definition 58) and $S_i^{(\nu)}$ as in (103).

Proof. The proof is similar as the proof of Lemma 70 and is based on an induction over $i = L, L - 1, ..., \ell$ as well. We adopt the notation from that proof.

- i = L: The assertion follows directly from (97).
- Assumption: Assertion holds up to an index i + 1:

$$\theta_k^{(\nu)} \le \lambda_4^{an_k - m_k} \left(\omega_2 2^{-k} \right)^{|\nu| + 2} + S_k^{(\nu)}, \quad \forall \nu : |\nu| < m_k, \quad \forall k = i + 1, i + 2, \dots, L.$$

• We first consider the case that $\sigma(t_i) = \{t_{i+1}\}$, i.e., $t_i = t_{i+1}$. This implies $n_i = n_{i+1} + 1$ and $n_i \ge 1$. Similar as in (111) one derives with $f_i^{(\nu)}$, $V_i^{(\nu)}$ as in (100), (101):

$$\theta_i^{(\nu)} \le \begin{cases} f_i^{(\nu)} + \theta_{i+1}^{(\nu)} & \forall \nu : |\nu| < m_{i+1}, \\ V_i^{(\nu)} & \forall \nu : m_{i+1} \le |\nu| < m_i. \end{cases}$$

In the upper case, we obtain (by using $an_{i+1} - m_{i+1} = an_i - m_i$)

$$\theta_i^{(\nu)} \leq f_i^{(\nu)} + \theta_{i+1}^{(\nu)} \leq f_i^{(\nu)} + \lambda_4^{an_{i+1} - m_{i+1}} \left(\omega_2 2^{-i-1}\right)^{|\nu| + 2} + S_{i+1}^{(\nu)} \leq \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} + S_i^{(\nu)}.$$

For the lower case, the quantity $V_i^{(\nu)}$ has to be estimated similarly as $\varepsilon_i^{(\nu)}$ in (113) by using (101), $\rho_{i+1} \leq \rho_i$, (113), and putting $q = \omega_2/(C_7\tilde{\omega})$:

$$V_i^{(\nu)} \le 2C_i \lambda_4^{an_{i+1}} \left(\tilde{\omega}\rho_i\right)^{|\nu|+2} {|\nu| \choose m_{i+1}+1} \le \lambda_4^{an_i-m_i} \left(\omega_2 2^{-i}\right)^{|\nu|+2} 2C_\Gamma \frac{(m_i+3)^{a+2}}{q^2(a-1)!} \left(\frac{\lambda_4}{q}\right)^{m_i-a}.$$

$$(117)$$

Provided $\lambda_4/q \leq 1/e$ and $q \geq \sqrt{2C_{\Gamma} \frac{(a+3)^{a+2}}{(a-1)!}}$ we obtain

$$\theta_i^{(\nu)} \le V_i^{(\nu)} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} + S_i^{(\nu)}. \tag{118}$$

This concludes the case of $t_{i+1} = t_i$.

It remains to consider $t_i \neq t_{i+1}$, i.e., $\rho_{i+1}/\rho_i \leq \bar{\rho} < 1$. We begin with estimating the sum in (102) by using the assumption of the induction:

$$\sum_{|\tilde{\nu}| < m_{i+1}} |\gamma_{\nu,\tilde{\nu},\tilde{c}}| \, \theta_{i+1}^{(\tilde{\nu})} \le \sum_{|\tilde{\nu}| < m_{i+1} \\ \tilde{\nu} \le \nu} {\nu \choose \tilde{\nu}} \rho_i^{|\nu-\tilde{\nu}|} \left(\lambda_4^{an_{i+1}-m_{i+1}} \left(\omega_2 2^{-i-1} \right)^{|\tilde{\nu}|+2} + S_{i+1}^{(\tilde{\nu})} \right). \tag{119}$$

We begin with considering the sum $S_i^{(\nu)}$ as in (103). A single summation term $f_k^{(\nu)}$ satisfies by putting $q = \omega_2/(C_7\tilde{\omega})$ and by using Assumption 42:

$$\begin{array}{lcl} f_k^{(\nu)} & = & C_{\Gamma} \lambda_4^{a n_{k+1} - m_{k+1}} \left(\tilde{\omega} \rho_k \right)^{|\nu| + 2} \\ & \leq & C_{\Gamma} \lambda_4^{a n_i - m_i} \left(\omega_2 2^{-i} \right)^{|\nu| + 2} \underbrace{\lambda_4^{a (n_{k+1} - n_i) + m_i - m_{k+1}} \left(\frac{2^{-k}}{q 2^{-i}} \right)^{|\nu| + 2}}_{=:\varphi} \end{array}$$

The quantity φ can be estimated by using $q \geq 2$ and $b \geq 2 (a \log \lambda_4 / \log 2 - 1)$

$$\varphi \le \lambda_4^{a(k+1-i)} \left(2^{i-k-1} \right)^{b+2} \le \lambda_4^{a(k+1-i)} 2^{2a(i-k-1)\log \lambda_4/\log 2} = \lambda_4^{-a(k+1-i)}$$

This leads to

$$S_i^{(\nu)} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} C_{\Gamma} \sum_{k=i}^{\infty} \lambda_4^{-a(k+1-i)} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} \frac{C_{\Gamma} \lambda_4^{-a}}{1 - \lambda_4^{-a}}.$$
(120)

Hence, as single term in the brackets of (119) can be estimated by

$${\binom{\nu}{\tilde{\nu}}} \rho_{i}^{|\nu-\tilde{\nu}|} \left(\lambda_{4}^{an_{i+1}-m_{i+1}} \left(\omega_{2} 2^{-i-1} \right)^{|\tilde{\nu}|+2} + S_{i+1}^{(\tilde{\nu})} \right) \leq \lambda_{4}^{an_{i}-m_{i}} \left(C_{7} 2^{-i} \right)^{|\nu|+2} {\binom{\nu}{\tilde{\nu}}} \times \left(\frac{\omega_{2}}{C_{7} 2} \right)^{|\tilde{\nu}|+2} \left(\frac{\lambda_{4}^{a}+C_{\Gamma}-1}{1-\lambda_{4}^{-a}} \right)$$

and the sum by

$$\left(\omega_2 2^{-i}\right)^{|\nu|+2} \lambda_4^{a n_i - m_i} \left(\frac{C_7}{\omega_2} + \frac{1}{2}\right)^{|\nu|} \frac{\lambda_4^a + C_\Gamma - 1}{4\left(1 - \lambda_4^{-a}\right)}$$

The condition $\omega_2 \geq 4C_7$ implies

$$\sum_{|\tilde{\nu}| < m_{i+1}} |\gamma_{\nu,\tilde{\nu},\tilde{c}}| \, \theta_{i+1}^{(\tilde{\nu})} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i} \right)^{|\nu| + 2} \left(\frac{3}{4} \right)^b \left(\frac{\lambda_4^a + C_{\Gamma} - 1}{4 \left(1 - \lambda_4^{-a} \right)} \right).$$

It remains to estimate $V_i^{(\nu)}$ in (102). Similarly as in (117), (118) we obtain,

- for
$$|\nu| < m_{i+1}$$
:

$$V_i^{(\nu)} \le f_i^{(\nu)} \le S_i^{(\nu)},$$

- for
$$m_{i+1} \le |\nu| < m_i$$
:

$$V_i^{(\nu)} \le \lambda_4^{an_i - m_i} \left(\omega_2 2^{-i}\right)^{|\nu| + 2} \bar{\rho}^b.$$

• Altogether, we have proved that the right-hand side in (102) satisfies

$$V_{i}^{(\nu)} + \sum_{|\tilde{\nu}| < m_{i+1}} |\gamma_{\nu,\tilde{\nu},\tilde{c}}| \,\theta_{i+1}^{(\tilde{\nu})} \leq \lambda_{4}^{an_{i}-m_{i}} \left(\omega_{2} 2^{-i}\right)^{|\nu|+2} \underbrace{\left(\frac{\lambda_{4}^{a} + C_{\Gamma} - 1}{4\left(1 - \lambda_{4}^{-a}\right)} \left(\frac{3}{4}\right)^{b} + \bar{\rho}^{b}\right)}_{=:\psi}$$

The condition

$$b \ge \max \left\{ \log \frac{\lambda_4^a + C_\Gamma - 1}{2\left(1 - \lambda_4^{-a}\right)} / \log \frac{4}{3}, \log 2 / \log \frac{1}{\bar{\rho}} \right\}$$

implies $\psi \leq 1$ yielding the proof.

Next, we will prove the representation formulae for $N_c^{(\nu)}$ and $\tilde{N}_c^{(\nu)}$ (cf. (95)).

Lemma 72 Let $N_c^{(\nu)}$, $\tilde{N}_c^{(\nu)}$ be as in (72), (94). Then, the representation and recursion formulae

$$\tilde{N}_{c}^{(\nu)}(x) = \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| \leq \tilde{m}} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}(x) + \sum_{|\tilde{\nu}| \leq \tilde{m} - 1} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \check{N}_{\tilde{c}}^{(\tilde{\nu})}(x)
N_{c}^{(\nu)}(x) = \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| \leq \tilde{m}} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \Phi_{\tilde{c}}^{\tilde{\nu}}(x) + \sum_{|\tilde{\nu}| \leq \tilde{m} - 1} \gamma_{\nu, \tilde{\nu}, \tilde{c}} N_{\tilde{c}}^{(\tilde{\nu})}(x)$$

hold.

Proof. Let $c \in T(\ell)$ and $|\nu| < m(\ell)$. Put $\tilde{m} = m(\ell + 1)$ and n = n(x). Leibnitz' rule for differentiation of products yields

$$\begin{split} \tilde{N}_{c}^{(\nu)}\left(x\right) &= \sum_{i=1}^{3} n_{i} \sum_{|\tilde{\nu}| \leq \tilde{m}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right) \frac{1}{\tilde{\nu}!} \partial^{\tilde{\nu}} \left[\check{\Phi}_{c}^{(\nu+e_{i})}\right] \left(M_{\tilde{c}}\right) \\ &= \sum_{|\tilde{\nu}| \leq \tilde{m}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right) \frac{1}{\tilde{\nu}!} \partial^{\tilde{\nu}} \left[\langle n, \cdot - M_{c} \rangle \check{\Phi}_{c}^{(\nu)}\right] \left(M_{\tilde{c}}\right) \\ &= \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| \leq \tilde{m}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right) \frac{1}{\tilde{\nu}!} \partial^{\tilde{\nu}} \left[\check{\Phi}_{c}^{(\nu)}\right] \left(M_{\tilde{c}}\right) \\ &+ \sum_{|\tilde{\nu}| \leq \tilde{m}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right) \sum_{i=1}^{3} \frac{n_{i}}{\tilde{\nu}!} \nu_{i} \partial^{\tilde{\nu}-e_{i}} \left[\check{\Phi}_{c}^{(\nu)}\right] \left(M_{\tilde{c}}\right) \\ &= \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| \leq \tilde{m}} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right) + \sum_{i=1}^{3} \sum_{|\tilde{\nu}| \leq \tilde{m}-1} n_{i} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu}+e_{i})}\left(x\right) \frac{1}{\tilde{\nu}!} \partial^{\tilde{\nu}} \left[\check{\Phi}_{c}^{(\nu)}\right] \left(M_{\tilde{c}}\right) \\ &= \langle n, M_{\tilde{c}} - M_{c} \rangle \sum_{|\tilde{\nu}| \leq \tilde{m}} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \check{\Phi}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right) + \sum_{|\tilde{\nu}| \leq \tilde{m}-1} \gamma_{\nu, \tilde{\nu}, \tilde{c}} \check{N}_{\tilde{c}}^{(\tilde{\nu})}\left(x\right). \end{split}$$

In the same fashion, the second recursion is proved.

Lemma 73 Let $\pi_i^{(\nu)}$ be as in (96), Then, the estimate

$$\pi_i^{(\nu)} \le \begin{cases} 0, & \forall \nu : |\nu| \le m_{i+1} - 1\\ C_i \rho_i^{|\nu|+2} \left(\frac{\rho_{i+1}}{\rho_i}\right)^{m_{i+1}+1} {|\nu| \choose m_{i+1}+1} & \forall \nu : m_{i+1} \le |\nu| \le m_i - 1 \end{cases}$$
(121)

holds with

$$C_i = C_{\Gamma} (m_{i+1} + 3)^3$$
.

Proof. $\tilde{\Phi}_{t_{i+1}}^{(\nu)}$ is the Taylor expansion of $\check{\Phi}_{t_i}^{(\nu)}|_{t_{i+1}}$ of order $\tilde{m}=m\,(i+1)$ about $M_{i+1}:=M_{t_{i+1}}$. Hence,

$$\pi_i^{(\nu)} = 0, \qquad \forall \nu : |\nu| \le \tilde{m} - 1.$$

We introduce the abbreviations

$$\check{\Phi}_{i+1}^{(\nu)} = \check{\Phi}_{t_{i}}^{(\nu)} \mid_{t_{i+1}}, \qquad \tilde{\Phi}_{i+1}^{(\nu)} = \tilde{\Phi}_{t_{i+1}}^{(\nu)}, \qquad n = n (y).$$

For $|\nu| \geq \tilde{m}$, the Taylor remainder $\Delta_c^{(\nu)} := \check{N}_c^{(\nu)} - \tilde{N}_{\tilde{c}}^{(\nu)}$ can be written in the form

$$\Delta_{i+1}^{(\nu)}(y) = \sum_{i=1}^{3} n_{j} \frac{\langle y - M_{i+1}, \nabla_{z} \rangle^{\tilde{m}+1}}{(\tilde{m}+1)!} \check{\Phi}_{i+1}^{(\nu+e_{j})}(z) = \frac{\langle y - M_{i+1}, \nabla_{z} \rangle^{\tilde{m}+1}}{(\tilde{m}+1)!} \langle n, z - M_{i} \rangle \check{\Phi}_{i+1}^{(\nu)}(z)$$

at an intermediate value $z = \xi = \xi(y) \in \overline{y, M_{i+1}}$. Applying Leibnitz' rule for differentiation of products results in

$$\Delta_{i+1}^{(\nu)}(y) = \langle n, \xi - M_i \rangle \frac{\langle y - M_{i+1}, \nabla_z \rangle^{\tilde{m}+1}}{(\tilde{m}+1)!} \check{\Phi}_{i+1}^{(\nu)}(z) + \langle n, y - M_{i+1} \rangle \frac{\langle y - M_{i+1}, \nabla_z \rangle^{\tilde{m}}}{\tilde{m}!} \check{\Phi}_{i+1}^{(\nu)}(z) .$$

The smoothness of the surface Γ implies that there exists C_{Γ} so that

$$|\langle n, \xi - M_i \rangle| \le C_{\Gamma} \rho_i^2, \qquad |\langle n, y - M_{i+1} \rangle| \le C_{\Gamma} \rho_{i+1}^2.$$

The derivatives can be estimated by

$$\left| \frac{\langle y - M_{i+1}, \nabla_z \rangle^{\tilde{m}+1}}{(\tilde{m}+1)!} \check{\Phi}_{i+1}^{(\nu)}(z) \right| = \left| \sum_{\substack{|\tilde{\nu}| = \tilde{m}+1\\ \tilde{\nu} \le \nu}} \binom{\nu}{\tilde{\nu}} \left(y - M_{i+1} \right)^{\tilde{\nu}} \left(z - M_i \right)^{\nu - \tilde{\nu}} \right|$$

$$(122)$$

$$\leq \sum_{\substack{|\tilde{\nu}|=\tilde{m}+1\\ \tilde{\nu}<\nu}} \binom{\nu}{\tilde{\nu}} \rho_i^{|\nu|-|\tilde{\nu}|} \rho_{i+1}^{|\tilde{\nu}|} \leq \rho_i^{|\nu|} \sum_{\substack{|\tilde{\nu}|=\tilde{m}+1\\ \tilde{\nu}<\nu}} \binom{\nu}{\tilde{\nu}} \left(\frac{\rho_{i+1}}{\rho_i}\right)^{|\tilde{\nu}|} = \rho_i^{|\nu|} \left(\frac{\rho_{i+1}}{\rho_i}\right)^{\tilde{m}+1} \sum_{\substack{|\tilde{\nu}|=\tilde{m}+1\\ \tilde{\nu}<\nu}} \binom{\nu}{\tilde{\nu}}.$$

Some combinatorial manipulations yield:

$$\sum_{\substack{|\tilde{\nu}|=\tilde{m}+1\\\tilde{\nu}\leq\nu}} \binom{\nu}{\tilde{\nu}} \leq \sum_{\substack{|\tilde{\nu}|=\tilde{m}+1\\\tilde{\nu}\leq\nu}} \binom{|\nu|}{|\tilde{\nu}|} \leq \binom{|\nu|}{\tilde{m}+1} \sum_{|\tilde{\nu}|=\tilde{m}+1} 1 = \frac{(\tilde{m}+3)(\tilde{m}+2)}{2} \binom{|\nu|}{\tilde{m}+1}. \tag{123}$$

Similarly,

$$\left| \frac{\langle y - M_{i+1}, \nabla_z \rangle^{\tilde{m}}}{\tilde{m}!} \check{\Phi}_{i+1}^{(\nu)}(z) \right| \leq \frac{(\tilde{m}+2)(\tilde{m}+1)}{2} \binom{|\nu|}{\tilde{m}} \rho_i^{|\nu|} \left(\frac{\rho_{i+1}}{\rho_i} \right)^{\tilde{m}}$$

is derived. Altogether, we have proved that

$$\pi_i^{(\nu)} = \left\| \Delta_{i+1}^{(\nu)} \right\|_{L^{\infty}(\tau)} \le \tilde{C} \rho_i^{|\nu|+2} \left(\frac{\rho_{i+1}}{\rho_i} \right)^{\tilde{m}+1} {|\nu| \choose \tilde{m}+1}$$

with
$$\tilde{C} = C_{\Gamma}(\tilde{m}+3)(\tilde{m}+2)(\tilde{m}+1)$$
.

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