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Hierarchical Quadrature for Multidimensional
Singular Integrals

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Hierarchical quadrature for multidimensional singular integrals

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Abstract

We introduce a method for the evaluation of singular integrals arising in the discretisation of integral equations. The method is based on the idea of repeated subdivision of domains. The integrals defined on these subdomains are classified. Each class can be expressed as a sum of regular integrals and representatives of other classes. A system of equations describes the relations between the classes. Therefore the approximate value of the singular integral only depends on the accuracy of the calculation of regular integrals.

AMS Subject Classifications: 65D32, 42B20.

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1 Introduction

We consider integrals as they arise in the discretisation of integral equations. In simplified notation, terms of the shape

$$\mathbb{I} = \int_{D^x} \int_{D^y} \|x-y\|^\alpha dy dx \quad \text{or} \quad \mathbb{I} = \int_{D^x} \int_{\partial D^y} \|x-y\|^\alpha dy dx \quad (1)$$

over domains $D^x, D^y \subset \mathbb{R}^n$ appear. In this paper we will restrict ourselves to arbitrary dimensions n for cubical and to $n \leq 3$ for simplicial domains.

If the distance between the domains D^x and D^y is strictly positive, \mathbb{I} is integrable for all α as the integral is not singular and can be evaluated exactly or treated by standard quadrature techniques [Str71], [CR93]. Likewise the integral is regular, if $\alpha \in 2\mathbb{N}_0$.

Therefore we want to consider the case $\alpha \in \mathbb{R} \setminus 2\mathbb{N}_0$ in which D^x and D^y share at least one common point. If $-1 < \alpha < 0$, the kernel function is improperly integrable. If $\alpha \leq -1$

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the integrals are strongly singular and \mathbb{I} has to be interpreted as a partie finie integral in the sense of Hadamard [Had52]. Our assumptions are explained for

$$\mathbb{I} = \int_{D^x} \int_{D^y} \kappa(x, y) dy dx \quad (2)$$

with a kernel κ satisfying particular assumptions.

All ideas given in this paper are based on the deliberations of [BH05], which depicts the given problem (1) for one-dimensional domains.

2 Basic definitions

The method described in this paper mainly exploits two characteristics of the integrand $\kappa(x, y)$. The first is the translation invariance and the second is the homogeneity of the kernel. Both are defined as follows.

Definition 2.1 (translational invariance)

A kernel $\kappa(x, y)$ is called *translational invariant*, if it satisfies

$$\kappa(x, y) = \kappa(x + c, y + c) \quad (c \in \mathbb{R}^n). \quad (3)$$

Definition 2.2 (homogeneity)

A kernel $\kappa(x, y)$ is called *homogeneous*, if it satisfies

$$\kappa(x, y) = s^g \kappa(sx, sy) \quad (s \in \mathbb{R}_{>0}), \quad (4)$$

where $g \in \mathbb{R}$ is the *degree of homogeneity*. Typically the parameters g and $-\alpha$ from (1) will coincide.

Furthermore, κ is assumed to be sufficiently smooth outside a neighbourhood of the possible singularity at $x = y$. A useful characterisation of the smoothness is given by the asymptotic smoothness (confer for instance [Hac09]).

Definition 2.3 (asymptotic smoothness)

The kernel $\kappa(x, y)$ is called *asymptotically smooth*, if there are constants $h_0, h_1 \in \mathbb{R}_{>0}$ such that

$$|\partial_x^v \partial_y^\mu \kappa(x, y)| \leq h_1 (h_0)^{|\nu+\mu|} (\mu + \nu)! \|x - y\|^{-g-|\nu+\mu|} \quad (5)$$

holds for all multi-indices $\nu \in \mathbb{N}_0^n, \mu \in \mathbb{N}_0^m$ and $g \in \mathbb{R}$ as mentioned in Definition 2.2.

Remark 2.4

We consider integrals as they arise in the discretisation of integral equations. Therefore we assume that the domains D^x, D^y originate from a regular grid without hanging nodes. Two domains can either have a positive distance, share a common face or are identical.

The next definition clarifies the designation of pairs of domains.

Definition 2.5 (regular and singular pairs of domains)

A pair of two domains is called *regular*, if the distance between them is strictly positive. Otherwise it is called *singular*. The dimension of the common face in the singular case is denoted by $d \geq 0$. The set of regular pairs is denoted by Γ_{reg} and the set of singular pairs sharing a common d -dimensional face is denoted by Γ_d .

Pairs of domains can be classified using equivalence classes. The underlying equivalence relation is defined next.

Definition 2.6 (equivalence of domains and of pairs of domains)

We call two domains $\rho, \sigma \subset \mathbb{R}^n$ *equivalent*, if a bijective transformation $\Phi: \mathbb{R}^n \rightarrow \mathbb{R}^n$ exists satisfying

$$\Phi(\sigma) = \rho \quad (6)$$

where Φ is a mapping given by

$$x = \Phi(\hat{x}) = t + c\mathbf{I}\hat{x} \quad (x \in \rho, \hat{x} \in \sigma),$$

with a constant vector $t \in \mathbb{R}^n$, a constant $c \in \mathbb{R}$ and the identity matrix \mathbf{I} . The transformation Φ allows scaling and translation of elements but no rotations.

Furthermore, we call two pairs of domains $\rho_1 \times \rho_2$ and $\sigma_1 \times \sigma_2$ *equivalent*, if

$$\begin{aligned} \Phi(\sigma_1) &= \rho_1, \\ \Phi(\sigma_2) &= \rho_2 \end{aligned} \quad (7)$$

holds with the same mapping Φ .

If the kernel κ is rotationally invariant or symmetric, the system of linear equations introduced in Sections 3.4 and 4.4 can be further simplified. The underlying definitions are given next.

Definition 2.7 (symmetry)

We denote $\kappa(x, y)$ as *symmetric*, if the symmetry condition

$$\kappa(x, y) = \kappa(y, x) \quad (\forall x, y \in \mathbb{R}^n) \quad (8)$$

holds.

Definition 2.8 (rotational invariance)

$\kappa(x, y)$ is called *rotationally invariant*, if

$$\kappa(x, y) = \kappa(\mathbf{R}x, \mathbf{R}y) \quad (9)$$

for all rotation matrices \mathbf{R} which represent rotations of $n \cdot \frac{\pi}{2}$ ($n \in \mathbb{Z}$) around the axes of the coordinate system.

$\kappa(x, y)$ is denoted as *partially rotationally invariant*, if the property mentioned above only holds for some axes.

3 Hypercubical domains

The hypercube or n -cube is the n -dimensional analogue of a square ($n = 2$) and a cube ($n = 3$). It can be described as the convex hull of its 2^n vertices. To represent the fact of cubical domains we slightly change the notation of (1) and write

$$\mathbb{I} = \int_{C^x} \int_{C^y} \|x - y\|^\alpha dy dx.$$

3.1 Local coordinates

Consider an arbitrary axis-aligned n -cube C given by its vertices $\{v_1, \dots, v_{2^n}\}$. The n -dimensional reference cube $\gamma^n := [0, 1]^n$ can be mapped to C via the formula

$$x = \Phi^C(\hat{x}) = v_1 + \mathbf{S}^C \hat{x} \quad (\hat{x} \in \gamma^n) \quad (10)$$

and an appropriately chosen scaling matrix \mathbf{S}^C depending on the difference $\bar{v}_1 - v_1$ with \bar{v}_1 being the opposite vertex of v_1 in the cube C . Now let Φ^{C^x} and Φ^{C^y} be mappings satisfying

$$C^x = \Phi^{C^x}(\gamma^n), \quad C^y = \Phi^{C^y}(\gamma^m).$$

Due to this notation we can transform the integral \mathbb{I} to an integral over n - and m -dimensional reference elements and write

$$\mathbb{I} = \int_{C^x} \int_{C^y} \|x - y\|^\alpha dy dx = c_1 \int_{\gamma^n} \int_{\gamma^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \quad (11)$$

with

$$\begin{aligned} \kappa_\gamma(\hat{x}, \hat{y}, \mathbf{v}^x, \mathbf{v}^y) &= \kappa(\Phi^{C^x}(\hat{x}) + \mathbf{v}^x, \Phi^{C^y}(\hat{y}) + \mathbf{v}^y) \\ &= \kappa(x + \mathbf{v}^x, y + \mathbf{v}^y) \quad (\mathbf{v}^x, \mathbf{v}^y \in \mathbb{R}^n) \end{aligned} \quad (12)$$

and c_1 being the product of the Jacobian determinants of Φ^{C^x} and Φ^{C^y} . We can now perform any of the following considerations on reference elements.

Remark 3.1

In general the kernel $\kappa_\gamma(\hat{x}, \hat{y}, 0, 0) = \kappa(\Phi^{C^x}(\hat{x}), \Phi^{C^y}(\hat{y})) = \kappa(v_1^{C^x} + \mathbf{S}^{C^x} \hat{x}, v_1^{C^y} + \mathbf{S}^{C^y} \hat{y})$ does not satisfy (4) as $v_1^{C^x} \neq v_1^{C^y}$, but in the singular case (cf. Definition 2.5) it will.

3.2 Splitting and labelling

Any n -cube C given by its vertices $\{v_1, \dots, v_{2^n}\}$ can be subdivided into 2^n subcubes:

$$\begin{aligned} C_1 &= \text{conv}\{v_1, v_{12}, \dots, v_{1,2^n}\} \\ C_2 &= \text{conv}\{v_{21}, v_2, v_{23}, \dots, v_{2,2^n}\} \\ &\vdots \\ C_{2^{n-1}} &= \text{conv}\{v_{2^{n-1},1}, \dots, v_{2^{n-1},2^{n-2}}, v_{2^{n-1}}, v_{2^{n-1},2^n}\} \\ C_{2^n} &= \text{conv}\{v_{2^n,1}, \dots, v_{2^n-1,2^n}, v_{2^n}\} \end{aligned}$$

with v_{ij} denoting the midpoint between two vertices v_i and v_j , $v_{ij} = \frac{v_i + v_j}{2}$.

Remark 3.2

Let $C^x \subset \mathbb{R}^n$ and $C^y \subset \mathbb{R}^m$ be two arbitrary hypercubes embedded in \mathbb{R}^n sharing a common d -dimensional face, so w.l.o.g.: $n \geq m \geq d \geq 0$ and $m > 0$, with a labelling as follows:

$$\begin{aligned} C^x &= \text{conv}\{v_1, \dots, v_{2^d}, v_{2^d+1}, \dots, v_{2^n}\}, \\ C^y &= \text{conv}\{v_1, \dots, v_{2^d}, v_{2^d+1}, \dots, v_{2^m}\}. \end{aligned}$$

Furthermore let these elements be subdivided according to the rules mentioned above. Then for the pairs $C_i^x \times C_i^y$, $i \in \{1, \dots, 2^d\}$, there exists a labelling such that these elements are equivalent to $C^x \times C^y$ with respect to Definition 2.6 using $c = \frac{1}{2}$.

Example 3.3

A possible labelling in the case of two cubes sharing a common 2-face is illustrated in Figure 1.

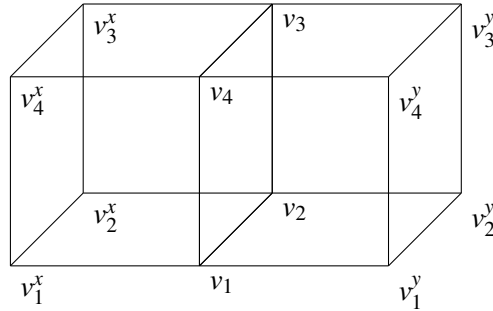


Figure 1: A possible labelling in the case of two cubes sharing a common 2-face

3.3 Computing the singular integral \mathbb{I}

Let $C^x \subset \mathbb{R}^n$ and $C^y \subset \mathbb{R}^m$ be two arbitrary hypercubes embedded in \mathbb{R}^n sharing a common d -dimensional face, so w.l.o.g.: $n \geq m \geq d \geq 0$ and $m > 0$,

$$\begin{aligned} C^x &= \text{conv}\{v_1, \dots, v_{2^d}, v_{2^d+1}, \dots, v_{2^n}\}, \\ C^y &= \text{conv}\{v_1, \dots, v_{2^d}, v_{2^d+1}, \dots, v_{2^m}\}. \end{aligned} \tag{13}$$

As already mentioned, the integration is defined on reference elements and mapped via (10) to $C^x \times C^y$. Subdividing the reference elements γ^n and γ^m according to Section 3.2 and expressing the integral \mathbb{I} as a sum over these subcubes yields

$$\mathbb{I} = c_1 \int_{\gamma^n} \int_{\gamma^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} = c_1 \sum_{i,j=1}^{2^n, 2^m} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \tag{14}$$

The integrals over the domains $\gamma_i^n \times \gamma_j^m$ with $i \in \{1, \dots, 2^d\}$ are singular (cf. Definition 2.5), since they share a common d -dimensional face. The pairings $\gamma_i^n \times \gamma_j^m$ with $i, j \in \{1, \dots, 2^d\}$, $i \neq j$, share common d^* -dimensional faces with $d^* \in \{0, \dots, d-1\}$. In the case of $i > 2^d$ or $j > 2^d$ the pairing is regular. Thus the integral \mathbb{I} is given by

$$\begin{aligned} \mathbb{I} &= c_1 \sum_{i=1}^{2^d} \int_{\gamma_i^n} \int_{\gamma_i^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &+ c_1 \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{\text{reg}}} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &+ c_1 \sum_{d^*=0}^{d-1} \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{d^*}} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \end{aligned} \quad (15)$$

The integrals over the pairings $\gamma_i^n \times \gamma_j^m$ with $i \in \{1, \dots, 2^d\}$ can be expressed in terms of \mathbb{I} exploiting the translation invariance (3) and the homogeneity (4) of the kernel, since

$$\begin{aligned} c_1 \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} &= c_1 \left(\frac{1}{2}\right)^{n+m} \int_{\gamma^n} \int_{\gamma^m} \kappa_\gamma\left(\frac{\hat{x}}{2}, \frac{\hat{y}}{2}, \mathbf{v}_{ii}, \mathbf{v}_{ii}\right) d\hat{y} d\hat{x} \\ &= c_1 \left(\frac{1}{2}\right)^{n+m+\alpha} \int_{\gamma^n} \int_{\gamma^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= \left(\frac{1}{2}\right)^{n+m+\alpha} \mathbb{I}, \end{aligned} \quad (16)$$

as the pairings $\gamma_i^n \times \gamma_j^m$, $i \in \{1, \dots, 2^d\}$, are equivalent to $\gamma^n \times \gamma^m$, if \mathbf{v}_{ii} is chosen in such a way that Remark 3.2 is valid.

Combining (15) and (16) we arrive at

$$\begin{aligned} \mathbb{I} &= 2^d c \mathbb{I} + c_1 \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{\text{reg}}} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &+ c_1 \sum_{d^*=0}^{d-1} \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{d^*}} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= \frac{c_1}{1 - 2^d c} \left(\sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{\text{reg}}} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \right. \\ &\quad \left. + \sum_{d^*=0}^{d-1} \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{d^*}} \int_{\gamma_i^n} \int_{\gamma_j^m} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \right) \end{aligned} \quad (17)$$

which is valid for constants

$$c = \left(\frac{1}{2}\right)^{n+m+\alpha}, \quad \alpha \neq -(n+m) + d.$$

The right-hand side of (17) contains only regular addends and singular ones with lower dimension of the common face. After a maximum of d applications of the method to

the remaining singular integrals, all singular parts can be expressed in terms of regular integrals.

Example 3.4 (integration over two identical cubes)

Let us consider the integral \mathbb{I} defined on two arbitrary but identical cubes $C^x = C^y = \text{conv}\{v_1, \dots, v_8\} \subset \mathbb{R}^3$ and a kernel function $\kappa(x, y)$ satisfying (3) and (4). We are interested in determining

$$\begin{aligned} \mathbb{I} &= \int_{C^x} \int_{C^y} \kappa(x, y) dy dx \\ &= c_1 \int_{\gamma^3} \int_{\gamma^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= c_1 \sum_{i,j=1}^8 \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \end{aligned}$$

Applying (17) for identical elements $\gamma_i^n = \gamma_j^m$ ($n = m = d = 3$) yields

$$\begin{aligned} \mathbb{I} &= \frac{c_1}{1-8c} \left(\sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_{\text{reg}}} \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \right. \\ &\quad + \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_0} \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &\quad + \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_1} \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &\quad \left. + \sum_{\gamma_i^n \times \gamma_j^m \in \Gamma_2} \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \right), \end{aligned}$$

with a constant $c = (\frac{1}{2})^{6+\alpha}$, $\alpha \neq -3$. The number of regular elements (Γ_{reg}) in the case of identical elements is zero, the case of common points (Γ_0) appears 8 times, the case of common edges (Γ_1) 24 times and the case of common faces (Γ_2) 24 times.

For the 24 common faces ($\gamma_i^3 \times \gamma_j^3 \in \Gamma_2$) the following is valid. In order not to overload the symbols, we will not change the notation except the additional index at \mathbb{I}_{ij} . The reader has to keep in mind that an additional step of transformation, namely the mapping of the reference element γ^3 to γ_i^3 and γ_j^3 resp., is necessary by which the shape of κ_γ and c_1 is altered.

$$\begin{aligned} \mathbb{I}_{ij} &= \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= \hat{c}_1 \int_{\gamma^3} \int_{\gamma^3} \hat{\kappa}_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= \hat{c}_1 \sum_{i,j=1}^8 \int_{\gamma_i^3} \int_{\gamma_j^3} \hat{\kappa}_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \end{aligned}$$

Applying (17) with $d = 2$ yields

$$\mathbb{I}_{ij} = \frac{\hat{c}_1}{1-4c} \left(\begin{aligned} & \sum_{\gamma_i^m \times \gamma_j^m \in \Gamma_{\text{reg}}} \int_{\gamma_i^3} \int_{\gamma_j^3} \hat{\mathbf{k}}_{\gamma}(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ & + \sum_{\gamma_i^m \times \gamma_j^m \in \Gamma_0} \int_{\gamma_i^3} \int_{\gamma_j^3} \hat{\mathbf{k}}_{\gamma}(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ & + \sum_{\gamma_i^m \times \gamma_j^m \in \Gamma_1} \int_{\gamma_i^3} \int_{\gamma_j^3} \hat{\mathbf{k}}_{\gamma}(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \end{aligned} \right),$$

which is valid for a constant $c = \left(\frac{1}{2}\right)^{6+\alpha}$ and $\alpha \neq -4$. In the case of a common face, Γ_1 contains 8 elements, Γ_0 4 elements and Γ_{reg} 48 elements. The shown procedure can be repeated for all singular cases. As we have to keep the cases of identical elements, common points, edges and faces in mind as well, we are restricted to $\alpha \notin \{-3, -4, -5, -6\}$.

Table 1 gives an overview of the appearing number of cases and the total number of regular integrals, if each singular case had to be treated independently. In the case of two common cubes, the subdivision method leads to 47880 regular pairs. Because of this, we will introduce equivalence classes to decrease the number of regular integrals and to be able to reuse already achieved results.

Table 1: Number of pairings and number of regular integrals for Example 3.4.

case of	number of					total number of regular pairs
	Γ_3	Γ_2	Γ_1	Γ_0	Γ_{reg}	
common cube:	8	24	24	8	0	47880
common face:		4	8	4	48	1788
common edge:			2	2	60	186
common point:				1	63	63

3.4 Simplification by equivalence classes

The method described in Section 3.3 is usable but inefficient if each regular integral is separately evaluated as shown in Table 1 of Example 3.4. Exploiting the properties (3) and (4), we are able to decrease the number of regular integrals and reuse already achieved results by using equivalence classes induced by the relation introduced in Definition 2.6.

Consider two arbitrary hypercubes $C^x \subset \mathbb{R}^n$ and $C^y \subset \mathbb{R}^m$ embedded in \mathbb{R}^n sharing a common d -dimensional face, w.l.o.g.: $n \geq m \geq d \geq 0$ and $m > 0$, as described in (13). If these two elements are subdivided as described in Section 3.2, N_{d^*} equivalence classes

can be described whose representatives share d^* -dimensional faces where $d^* \leq d$. The number N_{d^*} of these classes can be quantified via [Cox73]

$$N_{d^*} = 2^{d-d^*} \binom{d}{d^*}. \quad (18)$$

The number N of equivalence classes is therefore given by

$$N = \sum_{d^*=0}^d N_{d^*} = \sum_{d^*=0}^d 2^{d-d^*} \binom{d}{d^*}. \quad (19)$$

Now the solution can be described by a system of linear equations of the form $\mathbf{A}\hat{\mathbb{I}} = b$. Each row of the $N \times N$ -matrix $\mathbf{A} = a_{ij}$, $i, j=1 \dots N$ describes the representation of exactly one integral \mathbb{I}_i , $i = 1 \dots N$, defined on a representative of the class i in terms of all equivalence classes induced by the relation introduced in Definition 2.6. The diagonal and the off-diagonal elements read

$$\begin{aligned} a_{ii} &= 1 - 2^{d^*} c = 1 - 2^{d^*-n-m-\alpha}, \\ a_{ij} &= -n_{ij}c, \end{aligned} \quad (20)$$

where n_{ij} reflects how often the equivalence class j occurs in the representation of class i . The characteristics of the off-diagonal elements are only valid, if the reference elements are mapped to the elements, which means that an additional step of scaling may occur. If this step is skipped, additional scaling factors may appear in the matrix.

In this notation, the vector $\hat{\mathbb{I}}$ stores the values of the remapped representatives \mathbb{I}_i of the equivalence classes which have to be determined, and each entry of b collects the values of the sum of the regular integrals of the class in question.

Remark 3.5

By an appropriate sorting of the equivalence classes, a triangular structure of \mathbf{A} can be achieved.

Remark 3.6

If the kernel $\kappa(x, y)$ does not only fulfil (3) and (4), but is also symmetric and (partially) rotationally invariant as described in Definitions 2.7 and 2.8, the system can be further simplified. The potential of these simplifications are shown in Example 3.7 and 3.8.

Example 3.7 (simplified integration over two identical cubes)

Let us consider the same setting as given in Example 3.4, namely

$$\begin{aligned} \mathbb{I} &= \int_{C^x} \int_{C^y} \kappa(x, y) dy dx \\ &= c_1 \int_{\gamma^3} \int_{\gamma^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= c_1 \sum_{i,j=1}^8 \int_{\gamma_i^3} \int_{\gamma_j^3} \kappa_\gamma(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \end{aligned}$$

defined on two arbitrary but identical cubes $C^x = C^y \subset \mathbb{R}^3$ and a kernel function $\kappa(x, y)$ satisfying (3) and (4). Determining the number of equivalence classes for this configuration via (19) yields $N = 27$. This covers one case of identical elements, 6 common faces, 16 common edges and finally 8 common vertices. According to the numbers given in the Γ_{reg} -column of Table 1, now only 1800 regular integrals occur.

Example 3.8 (Example 3.7 with rotationally invariant kernel)

Let us now consider the same setting as in the example above but with the rotationally invariant kernel $\kappa = \frac{1}{\|x-y\|}$. In this case one has to consider 1 identical element, 1 common face, 1 common edge, 1 common vertex and only 171 regular integrals occur. To be more concrete, let $C^x = C^y = [0.5, 1]^3 \subset \mathbb{R}^3$. Due to (3) we define \mathbb{I} as follows,

$$\mathbb{I} = \int_{[0.5, 1]^3} \int_{[0.5, 1]^3} \frac{1}{\|x-y\|} dy dx = \int_{[0, 0.5]^3} \int_{[0, 0.5]^3} \frac{1}{\|x-y\|} dy dx.$$

The method shown in the previous sections leads to 27 equivalence classes. Due to the fact that the kernel is rotationally invariant, all classes with the same dimension in the common face can be conflated into one single class. So only four classes remain. Possible representatives are shown in Figure 2.

The matrix \mathbf{A} of the system of linear equations is given by (21). For the numbers n_{ij} confer Table 1.

$$\begin{aligned} \mathbf{A} &= \begin{pmatrix} 1 - 2^d c & -n_{12}c & -n_{13}c & -n_{14}c \\ & 1 - 2^{d^*}c & -n_{23}c & -n_{24}c \\ & & 1 - 2^{d^*}c & -n_{34}c \\ & & & 1 - 2^{d^*}c \end{pmatrix} \\ &= \begin{pmatrix} 0.75 & -0.75 & -0.75 & -0.25 \\ & 0.875 & -0.25 & -0.125 \\ & & 0.9375 & -0.0625 \\ & & & 0.96875 \end{pmatrix}. \end{aligned} \quad (21)$$

The reader has to keep in mind that the parameter d^* depends on the class in question. Row one holds the data for the identical elements ($d^* = d = 3$), row two represents elements with a common face ($d^* = 2$), row three is the common edge case ($d^* = 1$) and row four the common point case ($d^* = 0$). The parameter c is fixed with $c = \left(\frac{1}{2}\right)^{(n+m-\alpha)} = \left(\frac{1}{2}\right)^5$. The right-hand side b collects the values of the regular integrals of the class in question. The concrete values as well as c_{1j} , which represents the value c_1 of class j , depend on the chosen representatives of the equivalence classes. (22) lists the approximate values for the case of the elements shown in Figure 2 and the obtained solution $\hat{\mathbb{I}}$ for the equivalence classes. The first entry of $\hat{\mathbb{I}}$ is the approximate value for

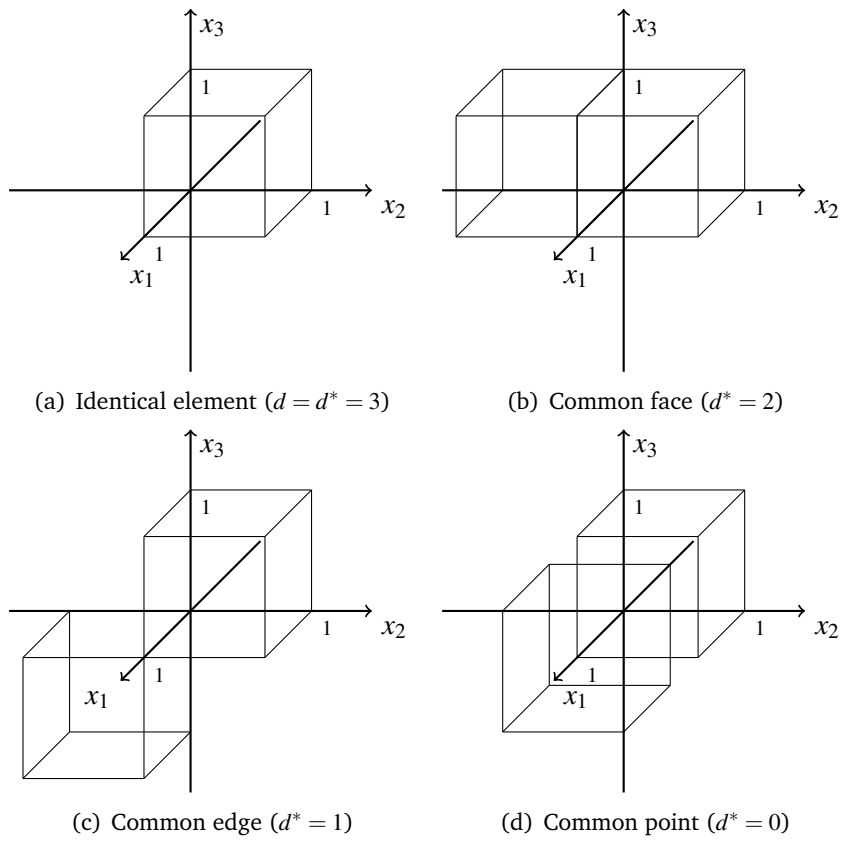


Figure 2: The representatives of the four equivalence classes of Example 3.8

the problem presented here.

$$b = \begin{pmatrix} 0 \\ 0.0190194 \\ 0.0196264 \\ 0.0175234 \end{pmatrix}, \quad \hat{\mathbb{I}} = \begin{pmatrix} 0.0588168 \\ 0.0306465 \\ 0.0221408 \\ 0.0180886 \end{pmatrix}. \quad (22)$$

4 Simplicial domains

As a second example this section covers domains of simplicial shape. The n -simplex is an n -dimensional analogue of a triangle or a tetrahedron. It is the convex hull of a set of $n + 1$ affinely independent points in Euclidean space of dimension n or higher. To represent the fact of domains with simplicial shape we change the notation of (1) as done in Section 3 and write

$$\mathbb{I} = \int_{T^x} \int_{T^y} \|x - y\|^\alpha dy dx.$$

In contrast to Section 3 we shall restrict ourselves to dimensions $n \leq 3$.

4.1 Local coordinates

Consider an arbitrary n -simplex T given by its corners $\{t_1, \dots, t_{n+1}\}$, $t_i \in \mathbb{R}^n$. The reference simplex $\tau \subset \mathbb{R}^n$, $\tau = \text{conv}\{0, e_1, \dots, e_n\}$, 0 denoting the origin and e_i the unit vectors of the Cartesian coordinate system, can be mapped to any given tetrahedron T via the formula

$$\begin{aligned} x &= \Phi^T(\hat{x}) = t_1 + \mathbf{J}^T \hat{x} \quad (\hat{x} \in \tau), \\ \mathbf{J}^T &= (t_2 - t_1, \dots, t_{n+1} - t_1). \end{aligned} \quad (23)$$

The superscripted T does not indicate the transpose. It is meant as an upper index.

Due to equation (23) we can repeat the procedure shown in Section 3.1 to transform the integral \mathbb{I} to an integral over n - and m -dimensional reference elements and write

$$\mathbb{I} = c_1 \int_{\tau^n} \int_{\tau^m} K_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \quad (24)$$

Here c_1 denotes the product of the Jacobian determinants of Φ^{T_x} , Φ^{T_y} and

$$\begin{aligned} \kappa_\tau(\hat{x}, \hat{y}, \mathbf{v}^x, \mathbf{v}^y) &= \kappa(\Phi^T(\hat{x}) + \mathbf{v}^x, \Phi^T(\hat{y}) + \mathbf{v}^y) \\ &= \kappa(x + \mathbf{v}^x, y + \mathbf{v}^y) \quad (\mathbf{v}^x, \mathbf{v}^y \in \mathbb{R}^n). \end{aligned} \quad (25)$$

Any of the following considerations can now be performed on reference elements.

Remark 4.1

In general, $t_1^{T_x} \neq t_1^{T_y}$ and hence κ is not homogeneous. In the singular case we have $t_1^{T_x} = t_1^{T_y}$ and equation (4) holds.

4.2 Splitting and labelling

Splitting simplices in arbitrary dimensions is not as straightforward as splitting hypercubes. So we restrict ourselves to dimensions $n \leq 3$ as already mentioned. The additional points t_{ij} which appear in the following are calculated via $t_{ij} = \frac{t_i + t_j}{2}$.

4.2.1 1-Simplex splitting (line)

An arbitrary line, given by $T = \text{conv}\{t_1, t_2\}$, can be subdivided into 2 lines

$$T_1 = \text{conv}\{t_1, t_{12}\}, \quad T_2 = \text{conv}\{t_{12}, t_2\}.$$

4.2.2 2-Simplex splitting (triangle)

A triangle $T = \text{conv}\{t_1, t_2, t_3\}$ can be decomposed into 4 triangles given by

$$\begin{aligned} T_1 &= \text{conv}\{t_1, t_{12}, t_{13}\}, & T_3 &= \text{conv}\{t_{13}, t_{23}, t_3\}, \\ T_2 &= \text{conv}\{t_{12}, t_2, t_{23}\}, & T_4 &= \text{conv}\{t_{12}, t_{13}, t_{23}\}. \end{aligned}$$

4.2.3 3-Simplex splitting (tetrahedron)

Any given tetrahedron $T = \text{conv}\{t_1, t_2, t_3, t_4\}$ can be subdivided into 8 subtetrahedra [Bey95]

$$\begin{aligned} T_1 &= \text{conv}\{t_1, t_{12}, t_{13}, t_{14}\}, & T_5 &= \text{conv}\{t_{12}, t_{13}, t_{14}, t_{24}\}, \\ T_2 &= \text{conv}\{t_{12}, t_2, t_{23}, t_{24}\}, & T_6 &= \text{conv}\{t_{12}, t_{13}, t_{23}, t_{24}\}, \\ T_3 &= \text{conv}\{t_{13}, t_{23}, t_3, t_{34}\}, & T_7 &= \text{conv}\{t_{13}, t_{14}, t_{24}, t_{34}\}, \\ T_4 &= \text{conv}\{t_{14}, t_{24}, t_{34}, t_4\}, & T_8 &= \text{conv}\{t_{13}, t_{23}, t_{24}, t_{34}\}. \end{aligned}$$

Remark 4.2

*In every case, the first $n + 1$ subelements are equivalent to T as they contain the corners of T , the remaining elements originate from the interior. In this setting, T_i is equivalent to T , if a labeling exists such that **J** in (6) holds with a constant $c = \frac{1}{2}$ (cf. Definition 2.6).*

Nevertheless a predication comparable to Remark 3.2 is not possible.

4.3 Computing the singular integral II

Let $T^x \subset \mathbb{R}^n$ and $T^y \subset \mathbb{R}^m$ be two arbitrary simplices embedded in \mathbb{R}^n which share a common d -dimensional face, w.l.o.g. $3 \geq n \geq m \geq d \geq 0$ and $m > 0$, given by their corners:

$$\begin{aligned} T^x &= \text{conv}\{t_1, \dots, t_{d+1}, t_{d+2}^{T_x}, \dots, t_{n+1}^{T_x}\}, \\ T^y &= \text{conv}\{t_1, \dots, t_{d+1}, t_{d+2}^{T_y}, \dots, t_{m+1}^{T_y}\}. \end{aligned} \tag{26}$$

As done in the previous sections, the integration is defined on reference elements and mapped to $T^x \times T^y$ by (23). The subdivision of reference elements τ^n , τ^m according to Section 4.2 yields an expression which reads

$$\mathbb{I} = c_1 \int_{\tau^n} \int_{\tau^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} = c_1 \sum_{i,j=1}^{2^n, 2^m} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \quad (27)$$

Now the singular parts in the sum on the right-hand side have to be identified. In dimensions $n > 1$, unfortunately not all singular elements $\tau_i^n \times \tau_j^m$ which share a common d -dimensional face can be expressed in terms of \mathbb{I} . So we have to distinguish different cases.

4.3.1 The cases of a common point or a common edge ($d = 0$ and $d = 1$)

In the case of a common 0- or a 1-dimensional face, the integrals defined on $\tau_1^n \times \tau_1^m$ and $\tau_1^n \times \tau_1^m$, $\tau_2^n \times \tau_2^m$, respectively, are singular in the sense of a common d -dimensional face. So we note:

$$\begin{aligned} d = 0: \quad \mathbb{I} &= c_1 \int_{\tau_1^n} \int_{\tau_1^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &\quad + c_1 \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{\text{reg}}} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}, \\ d = 1: \quad \mathbb{I} &= c_1 \int_{\tau_1^n} \int_{\tau_1^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} + c_1 \int_{\tau_2^n} \int_{\tau_2^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \quad (28) \\ &\quad + c_1 \sum_{\tau_i^n \times \tau_j^m \in \Gamma_0} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &\quad + c_1 \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{\text{reg}}} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}. \end{aligned}$$

In the case of a common point ($d = 0$) only the domain $\tau_1^n \times \tau_1^m$ is singular. All singular domains in the case of a common edge ($d = 1$) are listed in the following table. It includes the two 1-faces as well:

$$\begin{aligned} &\tau_1^n \times \tau_1^m, \tau_1^n \times \tau_2^m, \tau_1^n \times \tau_5^m, \tau_1^n \times \tau_6^m, \\ &\tau_2^n \times \tau_1^m, \tau_2^n \times \tau_2^m, \tau_2^n \times \tau_5^m, \tau_2^n \times \tau_6^m, \\ &\tau_5^n \times \tau_1^m, \tau_5^n \times \tau_2^m, \tau_5^n \times \tau_5^m, \tau_5^n \times \tau_6^m, \\ &\tau_6^n \times \tau_1^m, \tau_6^n \times \tau_2^m, \tau_6^n \times \tau_5^m, \tau_6^n \times \tau_6^m. \end{aligned}$$

As a closer look reveals, the integrals defined on $\tau_1^n \times \tau_1^m$ and $\tau_1^n \times \tau_1^m$, $\tau_2^n \times \tau_2^m$, respectively, can be expressed in terms of \mathbb{I} :

$$\begin{aligned} c_1 \int_{\tau_i^n} \int_{\tau_i^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} &= c_1 \left(\frac{1}{2}\right)^{n+m} \int_{\tau^n} \int_{\tau^m} \kappa_\tau\left(\frac{\hat{x}}{2}, \frac{\hat{y}}{2}, \mathbf{v}_{ii}, \mathbf{v}_{ii}\right) d\hat{y} d\hat{x} \\ &= c_1 \left(\frac{1}{2}\right)^{n+m-\alpha} \int_{\tau^n} \int_{\tau^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &= \left(\frac{1}{2}\right)^{n+m-\alpha} \mathbb{I}. \end{aligned}$$

This means, \mathbf{v}_{ii} is chosen in such a way that (7) holds with $c = \frac{1}{2}$. The combination of the upper identity with (28) yields directly

$$\begin{aligned} d = 0: \quad \mathbb{I} &= \frac{c_1}{1-c} \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{\text{reg}}} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x}, \\ d = 1: \quad \mathbb{I} &= \frac{c_1}{1-2c} \left(\sum_{\tau_i^n \times \tau_j^m \in \Gamma_0} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \right. \\ &\quad \left. + \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{\text{reg}}} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \right). \end{aligned} \quad (29)$$

The constant c equals $c = \left(\frac{1}{2}\right)^{n+m+\alpha}$. So the expressions are valid for $\alpha \neq -(n+m) + d$.

4.3.2 The case of a common face ($d = 2$)

The case of a common face ($d = 2$) is the first one, in which a singular element of dimension d appears, which cannot be expressed in terms of \mathbb{I} and therefore requires an additional splitting step.

Depending on the dimension of the subdivided elements τ^n and τ^m respectively, the following domains are singular in the sense of a common 2-dimensional face:

$$\begin{aligned} n = 2, m = 2: & \tau_1^2 \times \tau_1^2 \tau_2^2 \times \tau_2^2 \tau_3^2 \times \tau_3^2 \tau_4^2 \times \tau_4^2, \\ n = 3, m = 2: & \tau_1^3 \times \tau_1^2 \tau_2^3 \times \tau_2^2 \tau_3^3 \times \tau_3^2 \tau_6^3 \times \tau_4^2, \\ n = 3, m = 3: & \tau_1^3 \times \tau_1^3 \tau_2^3 \times \tau_2^3 \tau_3^3 \times \tau_3^3 \tau_6^3 \times \tau_6^3. \end{aligned}$$

The domains in the last column of the upper table are inequivalent to $\tau^n \times \tau^m$ (cf. Section 4.2). To simplify the notation we shall denote the inequivalent pairing by $\tau_\bullet^\circ \times \tau_\bullet^\circ$ and the according integral just by \mathbb{I}_\bullet regardless of the concrete labelling. The following table shows the domains τ_4^2 and τ_6^3 of the reference elements and the according transformations $\tau^\circ \rightarrow \tau_\bullet^\circ, \hat{x} \rightarrow \bar{x}$.

$$\tau_4^2 : \left\{ \begin{pmatrix} 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0.5 \end{pmatrix}, \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} \right\}, \quad \bar{x} = \begin{pmatrix} 0.5 \\ 0 \end{pmatrix} + \begin{pmatrix} -0.5 & 0 \\ 0.5 & 0.5 \end{pmatrix} \hat{x}$$

$$\tau_6^3 : \left\{ \begin{pmatrix} 0.5 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 0.5 \\ 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 0.5 \\ 0 \\ 0.5 \end{pmatrix} \right\},$$

$$\bar{x} = \begin{pmatrix} 0.5 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} -0.5 & 0 & 0 \\ 0.5 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{pmatrix} \hat{x}$$

The element τ_4^2 is shown in Figure 3 and a scaled and translated representative of element τ_6^3 is shown in Figure 4.

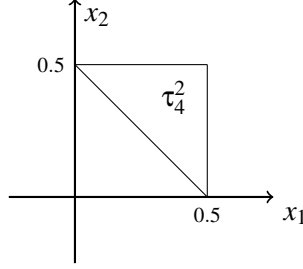


Figure 3: The domain τ_4^2

The element pair $\tau_\bullet^\circ \times \tau_\bullet^\circ$ is inequivalent to the reference element pair $\tau_\bullet^n \times \tau_\bullet^m$ but has the same dimension in the singular face. Therefore the elements τ_\bullet° require their own splitting according to Section 4.2. The repeated splitting yields pairs of domains which, if singular in the sense of a common d -dimensional face, are equivalent either to $\tau^n \times \tau^m$ or to $\tau_\bullet^n \times \tau_\bullet^m$. So the solution takes the form

$$\begin{aligned} \mathbb{I} &= 3c\mathbb{I} + \mathbb{I}_\bullet + c_1 \sum_{d^*=0}^{d-1} \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{d^*}} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &\quad + c_1 \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{\text{reg}}} \int_{\tau_i^n} \int_{\tau_j^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ \mathbb{I}_\bullet &= 3c\mathbb{I}_\bullet + c^2\mathbb{I} + c_1 \sum_{d^*=0}^{d-1} \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{d^*}} \int_{\tau_{\bullet,i}^n} \int_{\tau_{\bullet,j}^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \\ &\quad + c_1 \sum_{\tau_i^n \times \tau_j^m \in \Gamma_{\text{reg}}} \int_{\tau_{\bullet,i}^n} \int_{\tau_{\bullet,j}^m} \kappa_\tau(\hat{x}, \hat{y}, 0, 0) d\hat{y} d\hat{x} \end{aligned} \tag{30}$$

which can easily be rewritten as a system of linear equations $\mathbf{A}\hat{\mathbb{I}} = b$ where

$$\mathbf{A} = \begin{pmatrix} 1-3c & -c \\ -c & 1-3c \end{pmatrix}, \quad \hat{\mathbb{I}} = \begin{pmatrix} \mathbb{I} \\ \frac{1}{c}\mathbb{I}_\bullet \end{pmatrix}. \quad (31)$$

The right-hand side b collects the sum of the integral values with lower dimension in the singular face and the regular ones. The constant c is given as $c = \left(\frac{1}{2}\right)^{n+m+\alpha}$ and the determinant of \mathbf{A} equals $1 - 6c + 8c^2$. This restricts us to

$$\alpha \neq -(n+m) + 1 \text{ and } \alpha \neq -(n+m) + 2$$

as otherwise \mathbf{A} turns out to be singular.

Note that the second equation in (30) has been divided by c to obtain a more symmetric form of the matrix. This is necessary to adapt the notation with regard to equivalence classes.

4.3.3 The case of a common 3-face ($d = 3$)

The final and last configuration which can occur in the described setting is a common 3-dimensional face in the case of two identical tetrahedra. Splitting tetrahedra by the technique presented in Section 4.2 yields four elements which are equivalent to $\tau^n \times \tau^m$ and four elements which arise from the inner octahedron. They are not equivalent to other elements and therefore require a separate splitting. The resplitting reveals an additional element denoted by τ_s^2 which has to be splitted too. The five domains of interest are listed in Table 2 and shown in Figure 4. All elements have already been rescaled in such a way that the mapping of the reference elements does not require scaling.

An additional subdivision and resizing of the five elements that are inequivalent to $\tau^n \times \tau^m$ reveals a simple connection between the six classes which is reflected in the following system $\mathbf{A}\hat{\mathbb{I}} = b$ where

$$\mathbf{A} = \begin{pmatrix} 1-4c & -c & -c & -c & -c & 0 \\ -c & 1-4c & -c & -c & 0 & -c \\ -c & -c & 1-4c & 0 & -c & -c \\ -c & -c & 0 & 1-4c & -c & -c \\ -c & 0 & -c & -c & 1-4c & -c \\ 0 & -c & -c & -c & -c & 1-4c \end{pmatrix}, \quad \hat{\mathbb{I}} = \begin{pmatrix} \mathbb{I} \\ \frac{1}{c}\mathbb{I}_5 \\ \frac{1}{c}\mathbb{I}_6 \\ \frac{1}{c}\mathbb{I}_7 \\ \frac{1}{c}\mathbb{I}_8 \\ \frac{1}{c^2}\mathbb{I}_s \end{pmatrix}. \quad (32)$$

The right-hand side vector b again collects the sums of integrals defined on domains with lower-dimensional singular face. Please note the scaling of the rows 2 to 6 of \mathbf{A} as mentioned in the previous Section 4.3.2. Again c is given by $c = \left(\frac{1}{2}\right)^{3+3+\alpha}$ and the system is solvable with a unique solution for $\alpha \neq \{-3, -4, -5\}$.

Table 2: Domains not equivalent to τ^3

τ_5^3	:	{	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	}
τ_6^3	:	{	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	}
τ_7^3	:	{	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}$,	$\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	}
τ_8^3	:	{	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	}
τ_9^3	:	{	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}$,	$\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$,	$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	}

4.4 Simplification by equivalence classes

To reduce the number of regular integrals in the case of hypercubical domains, equivalence classes were introduced in Section 3.4. This is possible with simplices as well. The number of equivalence classes and hence the size of the system $\mathbf{A}\hat{\mathbf{l}} = b$ now does not only depend on the dimension of the singular face, but also on the dimension of the domains. The values for the configurations covered in this section are shown in the second column of Table 3.

The matrix takes a form similar to the one mentioned in (20), only the entries on the main diagonal may differ, as they reflect the presence of inequivalent elements.

Even though it is possible to attain further simplifications in the case of symmetric and (partially) rotationally invariant kernels, the achievements are not so massive as in the case of hypercubical domains as column three of Table 3 illustrates.

5 Integrals with polynomial kernels

To make use of the method described in this paper, we assume that the integrand $\kappa(x, y)$ is translationally invariant (3) and homogeneous (4).

If it is possible to decompose a non-translationally invariant kernel into sums of trans-

Table 3: The number of equivalence classes depending on n and $m = d$, resp., and the simplifications attained by symmetric and rotationally invariant kernels.

dimensions	number of d^* -dimensional pairs							
	unrotated				rotated			
	Γ_3	Γ_2	Γ_1	Γ_0	Γ_3	Γ_2	Γ_1	Γ_0
$n = 3, m = 3$	6	36	270	3348	4	12	109	1266
$n = 3, m = 2$		2	10	82		2	10	82
$n = 3, m = 1$			1	6			1	6
$n = 2, m = 2$		2	6	18		1	3	6
$n = 2, m = 1$			1	4			1	4
$n = 1, m = 1$			1	2			1	1

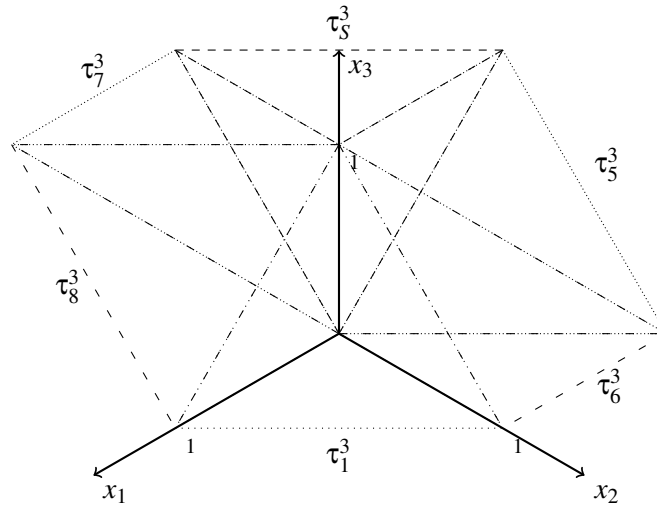


Figure 4: The domain τ_1^3 and the five domains appearing in the subdivision of τ_1^3 which are not equivalent to τ_1^3 .

lationally invariant parts, even such configurations can be handled. A simple example for such a case are kernels with a polynomial part like

$$\kappa(x, y) = \frac{p(x, y)}{\|x - y\|^{-\alpha}}. \quad (33)$$

By translating such a kernel, additional expressions are added to the polynomial $p(x, y)$, which may not be extractable depending on the degree of the polynomial. To transform the kernel into a sum of translational invariant parts, the binomial theorem can be used, as it splits a polynomial into a sum of monomials. By doing so the shape of the parameter c introduced in Sections 3 and 4 is altered, as the exponents of the monomials have to be taken into account. Let the multi-index η hold the exponents of the monomial in question. Then c is given by

$$c = \left(\frac{1}{2}\right)^{n+m+\alpha+\sum_{i=0}^n \eta_i}.$$

The principle is illustrated in the following example.

Example 5.1

Consider a double integral defined on $[0, 1] \times [0, 1]$ and a kernel $\kappa(x, y) = \frac{x^2}{\|x - y\|^{-\alpha}}$. So we are interested in the value of

$$\begin{aligned} \mathbb{I} &= \int_0^1 \int_0^1 \frac{x^2}{\|x - y\|^{-\alpha}} dy dx \\ &= \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \frac{x^2}{\|x - y\|^{-\alpha}} dy dx + \int_0^{\frac{1}{2}} \int_{\frac{1}{2}}^1 \frac{x^2}{\|x - y\|^{-\alpha}} dy dx \\ &\quad + \int_{\frac{1}{2}}^1 \int_0^{\frac{1}{2}} \frac{x^2}{\|x - y\|^{-\alpha}} dy dx + \int_{\frac{1}{2}}^1 \int_{\frac{1}{2}}^1 \frac{x^2}{\|x - y\|^{-\alpha}} dy dx. \end{aligned} \quad (34)$$

The first addend is equivalent to $\tau^1 \times \tau^1$ and the second covers the case of a common point. Both terms are unproblematic in the first step of decomposition, as only scaling is necessary and the translation does not affect the monomial:

$$\begin{aligned} \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \frac{x^2}{\|x - y\|^{-\alpha}} dy dx &= \left(\frac{1}{2}\right)^2 \int_0^1 \int_0^1 \frac{\left(\frac{x}{2}\right)^2}{\left\|\left(\frac{x}{2}\right) - \left(\frac{y}{2}\right)\right\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \int_0^1 \int_0^1 \frac{x^2}{\|x - y\|^{-\alpha}} dy dx \\ &= c\mathbb{I}, \\ \int_0^{\frac{1}{2}} \int_{\frac{1}{2}}^1 \frac{x^2}{\|x - y\|^{-\alpha}} dy dx &= \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \frac{x^2}{\|x - (y + \frac{1}{2})\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \int_0^1 \int_0^1 \frac{x^2}{\|x - y - 1\|^{-\alpha}} dy dx. \end{aligned}$$

Resplitting the case of a common point yields three regular elements and one which is equivalent to the element it originates from. The remaining parts of the sum (34) require the usage of the binomial theorem, which reads

$$(x+a)^d = \sum_{k=0}^d \binom{d}{k} x^k a^{d-k}.$$

Now the third addend which corresponds to the case of a common point, can be rewritten as

$$\begin{aligned} \int_{\frac{1}{2}}^1 \int_0^{\frac{1}{2}} \frac{x^2}{\|x-y\|^{-\alpha}} dy dx &= \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \frac{(x+\frac{1}{2})^2}{\|(x+\frac{1}{2})-y\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \int_0^1 \int_0^1 \frac{(x+1)^2}{\|x-y+1\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \sum_{k=0}^2 \binom{2}{k} 1^{2-k} \int_0^1 \int_0^1 \frac{x^k}{\|x-y+1\|^{-\alpha}} dy dx, \end{aligned}$$

requiring the solution of three cases of a common point but with different exponents k in the monomial. For all k we may write:

$$\begin{aligned} \int_0^1 \int_0^1 \frac{x^k}{\|x-y+1\|^{-\alpha}} dy dx &= \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \frac{x^k}{\|x-y+1\|^{-\alpha}} dy dx \\ &\quad + \int_0^{\frac{1}{2}} \int_{\frac{1}{2}}^1 \frac{x^k}{\|x-y+1\|^{-\alpha}} dy dx \\ &\quad + \int_{\frac{1}{2}}^1 \int_0^{\frac{1}{2}} \frac{x^k}{\|x-y+1\|^{-\alpha}} dy dx \\ &\quad + \int_{\frac{1}{2}}^1 \int_{\frac{1}{2}}^1 \frac{x^k}{\|x-y+1\|^{-\alpha}} dy dx. \end{aligned}$$

Only the second part of the upper sum is singular but it is equivalent to the source element it originates from. A similar way has to be used to rewrite the fourth part of the sum in (34), a case which is partially equivalent to \mathbb{I} .

$$\begin{aligned} \int_{\frac{1}{2}}^1 \int_{\frac{1}{2}}^1 \frac{x^2}{\|x-y\|^{-\alpha}} dy dx &= \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \frac{(x+\frac{1}{2})^2}{\|x-y\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \int_0^1 \int_0^1 \frac{(x+1)^2}{\|x-y\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \sum_{k=0}^2 \binom{2}{k} 1^{2-k} \int_0^1 \int_0^1 \frac{x^k}{\|x-y\|^{-\alpha}} dy dx \\ &= \left(\frac{1}{2}\right)^{2+\alpha+2} \mathbb{I} \\ &\quad + \left(\frac{1}{2}\right)^{2+\alpha+2} \sum_{k=0}^1 \binom{2}{k} 1^{2-k} \int_0^1 \int_0^1 \frac{x^k}{\|x-y\|^{-\alpha}} dy dx. \end{aligned}$$

The configurations for $k = 0$ and $k = 1$ can be treated by the same method as described to obtain an appropriate splitting. Each splitting only depends on equivalence classes of the same or lower degree in the monomial. This holds in general for the cases of a d -dimensional face as well.

6 Uncovered parameter configurations

The method described in Sections 3 and 4 is not usable for certain hypersingular integrals. For example, if an n -dimensional and an m -dimensional hypercube share a d -dimensional face, we are restricted to $\alpha \neq -(n + m) + d^*$, $\forall d^* = d \dots 0$.

In the case of $n = m = 1$, [BH05] presents a solution of the problem in the form of an alternative splitting strategy. This is based on the concept of Hadamard integrals and cannot be generalised to higher dimensions as it would require the use of curved subdomains.

7 Approximation of the regular integrals and quadrature error estimation

7.1 Theoretical estimates

As described in the introduction and mentioned in Definition 2.3, we assume that the kernel κ is asymptotically smooth outside a neighbourhood of the possible singularity of order $g \in \mathbb{R}_{\geq 0}$ at $x = y$. So we expect the existence of constants $h_0, h_1 \in \mathbb{R}_{>0}$ such that

$$|\partial_x^v \partial_y^\mu \kappa(x, y)| \leq h_1 (h_0)^{|\nu + \mu|} (\mu + \nu)! \|x - y\|^{-g - |\nu + \mu|} \quad (35)$$

holds for all multi-indices $\nu \in \mathbb{N}_0^n$ and $\mu \in \mathbb{N}_0^m$. Typically the parameters $-\alpha$ and g from (4) will coincide. This expression can be rewritten to reflect the given geometric situation, so it reads

$$\|\partial_x^v \partial_y^\mu \kappa(x, y)\|_{\infty, D_i^x \times D_j^y} \leq \frac{h_1}{\delta_{ij}^g} \left(\frac{h_0}{\delta_{ij}}\right)^{|\nu + \mu|} (\mu + \nu)!, \quad (36)$$

$\delta_{ij} := \text{dist}(D_i^x, D_j^y)$, for all settings where $D_i^x \cap D_j^y = \emptyset$. If we now apply Theorem 3.2 of [BG04] to the standard tensor product Chebyshev interpolation operator in dimension d and combine this with (36) we obtain an expression which reads

$$\|\kappa - k\|_{\infty, D_i^x \times D_j^y} \leq \frac{8eh_1(2p)^{d+1}}{\delta_{ij}^g} \left(1 + \frac{h_0 \rho_{ij}}{\delta_{ij}}\right) \left(1 + \frac{2\delta_{ij}}{h_0 \rho_{ij}}\right)^{-2p},$$

$\rho_{ij} := \text{diam}(D_i^x \times D_j^y)$, including the Euler number e and $k \in \mathbb{P}_{2p-1}$, where \mathbb{P}_{2p-1} denotes the space of tensor product polynomials of order $2p - 1$. This can be rewritten as

$$\|\kappa - k\|_{\infty, D_i^x \times D_j^y} \leq \frac{8eh_1(2p)^{d+1}}{\delta_{ij}^g} \left(1 + \frac{h_0 \rho_{ij}}{\delta_{ij}}\right) \left(\frac{h_0 \rho_{ij}}{h_0 \rho_{ij} + 2\delta_{ij}}\right)^{2p}. \quad (37)$$

Up to this point, the given equations do not require approximation. All expressions hold for exact values. But it is possible to replace the exact integrals by their approximations. We denote this by $Q(\mathbb{I})_{D_i^x \times D_j^y}$ in contrast to the exact integrals $\mathbb{I}_{D_i^x \times D_j^y}$. With $\mathbb{I}_{D_i^x \times D_j^y}$ we denote both the integral and its value.

Let $Q(\mathbb{I})_{D_i^x \times D_j^y}$ be a method defined on $D_i^x \times D_j^y$, which is exact for tensor product polynomials of order $2p - 1$. For example the tensor product Gauss quadrature fulfils this for both cubical and simplicial domains [Str71].

As the method is exact for $k \in \mathbb{P}_{2p-1}$, the expression

$$\left\| \mathbb{I}_{D_i^x \times D_j^y} - Q(\mathbb{I})_{D_i^x \times D_j^y} \right\| \leq 2 \min_{k \in \mathbb{P}_{2p-1}} \| \kappa - k \|_{\infty, D_i^x \times D_j^y}$$

is valid. In conjunction with (37) this last expression yields the estimate

$$\left\| \mathbb{I}_{D_i^x \times D_j^y} - Q(\mathbb{I})_{D_i^x \times D_j^y} \right\| \leq C(p) \left(\frac{h_0 \rho_{ij}}{h_0 \rho_{ij} + 2\delta_{ij}} \right)^{2p} \quad (38)$$

and $C(p) = \frac{16eh_1(2p)^{d+1}}{\delta_{ij}^g} \left(1 + \frac{h_0 \rho_{ij}}{\delta_{ij}} \right)$. As $\delta_{ij} := \text{dist}(D_i^x, D_j^y) > 0$ for regular integrals, the quadrature error converges exponentially in the order p .

The right-hand side b of the system of linear equations mentioned in Sections 3.4 and 4.4 collects only regular integrals of shape $\mathbb{I}_{\ell, D_i^x, D_j^y}$ for the ℓ -th equivalence class. We denote the maximal approximation error by

$$\varepsilon := \max_{\substack{1 \leq \ell \leq N \\ D_i^x \cap D_j^y = \emptyset}} \left\{ \left\| \mathbb{I}_{\ell, D_i^x \times D_j^y} - Q(\mathbb{I})_{\ell, D_i^x \times D_j^y} \right\| \right\}. \quad (39)$$

Because (38) holds for all regular integrals, it is valid for ε as well:

$$\varepsilon \leq \frac{16eh_1(2p)^{d+1}}{\delta_{ij}^g} \left(1 + \frac{h_0 \rho_{ij}}{\delta_{ij}} \right) \left(\frac{h_0 \rho_{ij}}{h_0 \rho_{ij} + 2\delta_{ij}} \right)^{2p}.$$

The error of approximation for the singular integrals can now be bounded in the following way:

$$\| \mathbb{I}_i - Q(\mathbb{I}_i) \| \leq c(\mathbf{A}) \varepsilon$$

with a constant $c(\mathbf{A})$, as the matrix \mathbf{A} is constant with respect to the integration.

7.2 Numerical experiments

Finally we present the results of some numerical experiments. First, we choose as domain the reference cube $\gamma^3 = [0, 1]^3 \subset \mathbb{R}^3$. The integral takes the form

$$\mathbb{I} = \int_{\gamma^3} \int_{\gamma^3} \frac{x_1^{v_1} x_2^{v_2} x_3^{v_3} y_1^{\mu_1} y_2^{\mu_2} y_3^{\mu_3}}{\|x - y\|^1} dy dx. \quad (40)$$

For such a configuration an exact solution can be obtained by [Hac02]. Table 4 presents relative errors and the total number of kernel evaluations (in brackets) depending on the degree of the numerator monomial of (40) and the number of Gauss points p using the simplifications given by symmetry and rotation of elements where possible.

Second, we choose as domain the reference simplex $\tau^3 = \{0, e_1, e_2, e_3\} \subset \mathbb{R}^3$, 0 denoting the origin and e_i the unit vectors of the Cartesian coordinate system. Now the integral takes the form

$$\mathbb{I} = \int_0^1 \int_0^{1-x_1} \int_0^{1-x_1-x_2} \int_0^1 \int_0^{1-y_1} \int_0^{1-y_1-y_2} \frac{x_1^{v_1} x_2^{v_2} x_3^{v_3} y_1^{\mu_1} y_2^{\mu_2} y_3^{\mu_2}}{\|x-y\|^2} dy dx. \quad (41)$$

As for such a configuration no exact solution is given, we calculate numerical results using the method described in Section 4. The appearing regular integrals are approximated by Gaussian integration of order 19 using $p = 10$ Gauss points. The obtained values for lower number of Gauss points are compared to these values. The relative errors and the total number of kernel evaluations (in brackets) using the simplifications given by symmetry and rotation of elements where possible are given in Table 5.

Table 4: Relative errors and number of kernel evaluations (in brackets) for different degrees of the numerator monomial and number of Gauss points on cubical domains.

$v_1 \dots \mu_3$	$p=1$	2	3	4	5	6	7
000000	1.438 ₋₀₄ (171)	9.267 ₋₀₅ (10,944)	5.390 ₋₀₉ (124,659)	1.767 ₋₀₉ (700,416)	3.476 ₋₁₃ (2,671,875)	6.444 ₋₁₃ (7,978,176)	2.465 ₋₁₄ (20,117,979)
000001	1.438 ₋₀₄ (450)	9.267 ₋₀₅ (28,800)	5.390 ₋₀₉ (328,050)	1.767 ₋₀₉ (1,843,200)	3.476 ₋₁₃ (7,031,250)	6.446 ₋₁₃ (20,995,200)	2.477 ₋₁₄ (52,942,050)
000002	6.719 ₋₀₃ (729)	8.821 ₋₀₅ (46,656)	7.060 ₋₀₈ (531,441)	1.781 ₋₀₉ (2,985,984)	1.294 ₋₁₁ (11,390,625)	8.498 ₋₁₃ (34,012,224)	2.895 ₋₁₄ (85,766,121)
000123	2.108 ₋₀₂ (5,376)	7.774 ₋₀₅ (344,064)	2.191 ₋₀₇ (3,919,104)	1.837 ₋₀₉ (22,020,096)	3.602 ₋₁₁ (84,000,000)	1.230 ₋₁₂ (250,822,656)	1.266 ₋₁₄ (63,2481,024)
012012	2.351 ₋₀₂ (11,052)	1.478 ₋₀₄ (707,328)	4.651 ₋₀₇ (8,056,908)	3.096 ₋₀₉ (45,268,992)	8.499 ₋₁₁ (172,687,500)	2.392 ₋₁₂ (515,642,112)	9.544 ₋₁₅ (1,300,256,748)
123123	4.498 ₋₀₂ (155,472)	2.495 ₋₀₄ (9,950,208)	1.586 ₋₀₆ (113,339,088)	5.418 ₋₀₉ (636,813,312)	2.480 ₋₁₀ (2,429,250,000)	3.724 ₋₁₂ (7,253,701,632)	4.300 ₋₁₃ (18,291,125,328)

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Table 5: Relative errors and number of kernel evaluations (in brackets) for different degrees of the numerator monomial and number of Gauss points on simplicial domains.

$\nu_1 \dots \mu_3$	$p=1$	2	3	4	5	6	7
000000	4.352 ₋₀₁ (85,194)	4.015 ₋₀₃ (5,452,416)	2.632 ₋₀₅ (62,106,426)	5.490 ₋₀₆ (348,954,624)	3.667 ₋₀₇ (1,331,156,250)	9.379 ₋₀₉ (3,974,811,264)	2.373 ₋₀₈ (10,022,988,906)
000001	4.335 ₋₀₁ (290,904)	4.125 ₋₀₃ (18,617,856)	2.875 ₋₀₆ (212,069,016)	2.851 ₋₀₆ (1,191,542,784)	5.533 ₋₀₈ (4,545,375,000)	3.593 ₋₀₈ (13,572,417,024)	2.147 ₋₀₈ (34,224,564,696)
000002	4.354 ₋₀₁ (496,614)	5.110 ₋₀₃ (31,783,296)	1.762 ₋₀₆ (362,031,606)	2.424 ₋₀₆ (2,034,130,944)	3.797 ₋₀₈ (7,759,593,750)	5.410 ₋₀₈ (23,170,022,784)	2.251 ₋₀₈ (58,426,140,486)

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