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Abstract

In boundary element methods, the evaluation of the weakly singular integrals can be performed either a) numerically, b) symbolically, i.e., by explicit expressions, or c) in a combined manner. The explicit integration is of particular interest, when the integrals contain the singularity or if the singularity is rather close to the integration domain.

We describe the explicit expressions for the sixfold volume integrals arising for the Newton potential, i.e., for a $1/r$ integrand. The volume elements are axi-parallel bricks. The sixfold integrals are typical for the Galerkin method. However, the threefold integral arising from collocation methods can be derived in the same way.

Furthermore, this report contains a description of the program together with examples for its use.

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1 Introduction

The evaluation of the Newton potential is an often needed task in integral equations. We consider a Galerkin formulation with cubes (or more generally bricks) as finite elements. Then, in the 3D case, we have to determine the six-fold integrals

$$I(B',B'') := \iiint\limits_{B'} \left(\iiint\limits_{B''} \frac{x_1^{\nu_1} x_2^{\nu_2} x_3^{\nu_3} y_1^{\mu_1} y_2^{\mu_2} y_3^{\mu_3}}{\sqrt{(x_1-y_1)^2+(x_2-y_2)^2+(x_3-y_3)^2}} dy_1 dy_2 dy_3 \right) dx_1 dx_2 dx_3, \tag{1.1}$$

where B' and B'' are Cartesian bricks

$$B' = \prod_{i=1}^{3} [a_i', b_i'] \qquad \text{and } B'' = \prod_{i=1}^{3} [a_i'', b_i''] \,. \tag{1.2}$$

The monomials in the numerator are due to higher order finite element functions and can be replaced by any polynomial in x_i, y_i $(i = 1, 2, 3)$.

The goal of the approach in this paper is a multiple one.

- If the boxes B', B'' have a distance comparable with their diameters, the integral (1.1) can be determined by expansions of the kernel. This leads, e.g., to the efficient panel clustering method for the matrix-vector multiplication (cf. [5], [10]) or to the hierarchical matrix technique (cf. [3], [4]). However, for neighbouring boxes as, e.g., in (1.3) below, accurate numerical approximations are more involved. In this case, an exact representation is of interest. Nevertheless, numerical approximations are possible (see, e.g., [1], [6], [7], [10]-[14]).
- In the case of sparse grids, integrals like (1.1) occur for possibly elongated but intersecting boxes (take for instance $B' = [0, 100] \times [0, 1] \times [0, 1]$ and $B'' = [0, 1] \times [0, 100] \times [0, 1]$, cf. §3.15 and §6.10). Again, an accurate numerical approximation is possible but more involved, in particular, if a certain quadrature error bound is to be guaranteed.

- Due to the exponents ν_i and μ_i, we may apply (1.1) to higher-order polynomials as they appear in the *hp*-method. In that case the expected exponential convergence requires extremely accurate quadrature results which are much more costly than in the case of *h*-methods (cf. [14]).

- In applications of the above mentioned hierarchical matrix technique to a very anisotropic grid, there is interest in antiderivatives with respect to some of the variables appearing in (1.1). Since in this case one is interested in the singularity behaviour with respect to the remaining variables, one needs the symbolic representations offered by this paper.

Problem (1.1) is solved by providing the antiderivatives of the integrand with respect to the six variables in the order $x_1, y_1, x_2, y_2, x_3, y_3$. Therefore, the results can also be used of 1D or 2D integration problems

$$\int_{I'}\int_{I''} \frac{x^\nu y^\mu}{\sqrt{(x-y)^2 + A^2}} dx dy, \qquad \iint_{R'}\iint_{R''} \frac{x_1^{\nu_1} x_2^{\nu_2} y_1^{\mu_1} y_2^{\mu_2}}{\sqrt{(x_1-y_1)^2 + (x_2-y_2)^2 + A^2}} dx_1 dy_1 dx_2 dy_2$$

over intervals I', I'' or rectangles R', R'', where A is a constant. The case of other elements than rectangles is discussed in Remark 3.6. The partial results after less than six integrations are of interest, if the direct integration with respect to the first variable should be combined with a numerical one for the remaining variables.

Of course, one can find results about antiderivatives here and there in the literature, e.g., [9, p.122] contains formulae for the piecewise constant case ($\nu_i = 0$) and collocation (i.e., only x-integration, no y-integration).

As mentioned above, the integral (1.1) can be approximated by the panel clustering method if the bricks B', B'' have a sufficient distance. However, there remain at least the following cases which are taken as test examples in §3.14: 1) $B' = B''$, 2) B', B'' have a common face, 3) B', B'' have a common edge, and 4) B', B'' have a common vertex. Then the distance is zero and a singularity appears in the denominator of (1.1). Since (1.1) is translation invariant, we may assume that B' has a vertex at the origin. Further, due to a simple scaling, $[a_1', b_1'] = [0,1]$ may be assumed. Therefore, $B' = [0,1]^3$ may be assumed if B' is a cube. In each step of the integration (construction of antiderivatives) in the order $x_1, y_1, x_2, y_2, x_3, y_3$, the general analysis is illustrated by the example of (1.1) for piecewise constant finite elements and face-neighboured unit cubes, i.e.,

$$\nu_i = \mu_i = 0, \quad B' = [0,1]^2 \times [1,2], \quad B'' = [0,1]^3. \tag{1.3}$$

The antiderivatives are obtained by recursion formulae, which are compactly collected in the final section §5.

The appendix contains hints how to use the program producing these results. The source text of the program are obtainable from `http://www.mis.mpg.de/scicomp/wh_artikel.html`

2 Functions needed for the Representation

When we perform the integration with respect x_i, y_i, the other variables are considered as constants, so that we consider typically a function of x, y (replacing x_i, y_i) only. We use the following notation for the constants, which are variable for other i:

$$\begin{array}{ll} X := x_1 - y_1, & \Xi := Y^2 + Z^2, \\ Y := x_2 - y_2, & \Upsilon := X^2 + Z^2, \\ Z := x_3 - y_3, & \Theta := X^2 + Y^2. \end{array} \tag{2.1}$$

The functions that appear during the integration process are listed below.

We start with the integrand

$$F_{k,l}(x, y; \Xi) = \frac{x^k y^l}{\sqrt{(x-y)^2 + \Xi}} \qquad \text{with } \Xi \geq 0. \tag{2.2}$$

The integers k, l will always indicate numbers from $\mathbb{N}_0$. Although $\Xi \geq 0$ is a general non-negative real number, its meaning is seen from (2.1), provided that $x = x_1$ and $y = y_1$.

The first and second integration leads to the functions[1]

$$G_{k,l}(x,y;\Xi) = x^k y^l \sqrt{(x-y)^2 + \Xi}\,, \tag{2.3}$$

$$L_{k,l}(x,y;\Xi) = x^k y^l \ln\left(x - y + \sqrt{(x-y)^2 + \Xi}\right). \tag{2.4}$$

Fixing the values of $x = x_1$ and $y = y_1$ and interpreting the functions from above as function of $x = x_2$ and $y = y_2$ (appearing in Ξ) give rise to

$$M_{k,l}\,(x,y;X,Z) = x^k y^l \ln\left(X + \sqrt{(x-y)^2 + \Upsilon}\right) \qquad \text{with } \Upsilon = X^2 + Z^2. \tag{2.5}$$

The x_2-integration uses

$$A_{kl}\,(x,y;X,Z) = \frac{x^k y^l}{\sqrt{(x-y)^2+\Upsilon}\left(X + \sqrt{(x-y)^2+\Upsilon}\right)}, \tag{2.6}$$

$$B_{k,l}\,(x,y;X,Z) = \frac{x^k y^l}{Z}\left(\arctan\frac{x-y}{Z} - \arctan\left(\frac{X}{Z}\frac{x-y}{\sqrt{(x-y)^2+\Upsilon}}\right)\right) \quad \text{with } \Upsilon = X^2+Z^2,$$

$$P_{k,l}(x,y) = x^k y^l.$$

The interpretation of the function $B_{k,l}$ as function of $x = x_3$ and $y = y_3$ (appearing in Z) will give rise to[2]

$$C_{k,l}\,(x,y;X,Y) = x^k y^l\,(x-y)\left(\arctan\frac{(x-y)\sqrt{\Theta+(x-y)^2}}{XY} - \arctan\frac{x-y}{Y}\right) = C''_{k,l} - C'_{k,l} \tag{2.7}$$

with $\Theta = X^2 + Y^2$ and

$$C'_{k,l}\,(x,y;Y) = x^k y^l\,(x-y)\arctan\frac{x-y}{Y} = (x-y)\,Q_{k,l}(x,y;Y), \tag{2.8}$$

$$\begin{aligned} C''_{k,l}\,(x,y;X,Y) &= x^k y^l\,(x-y)\arctan\frac{(x-y)\sqrt{\Theta+(x-y)^2}}{XY} = C^+_{k,l} + C^-_{k,l} \text{ with} \\ C^+_{k,l}\,(x,y;X,Y) &= (x-y)\,R^+_{k,l}(x,y;X,Y), \\ C^-_{k,l}\,(x,y;X,Y) &= (x-y)\,R^-_{k,l}(x,y;X,Y) = C^+_{k,l}\,(x,y;Y,X)\,, \end{aligned} \tag{2.9}$$

where $Q_{k,l}$ and $R^{\pm}_{k,l}$ are defined in

$$\begin{aligned} Q_{k,l}\,(x,y;Y) &= x^k y^l \arctan\frac{x-y}{Y}, \\ R^+_{k,l}(x,y;X,Y) &= x^k y^l \arctan\left(\frac{Y}{X}\frac{x-y}{\sqrt{\Theta+(x-y)^2}}\right),\ \Theta = X^2+Y^2, \\ R^-_{k,l}(x,y;X,Y) &= x^k y^l \arctan\left(\frac{X}{Y}\frac{x-y}{\sqrt{\Theta+(x-y)^2}}\right). \end{aligned} \tag{2.10}$$

[1] $G_{k,l}$ could be expressed by $F_{k,l}$ via $G_{k,l}(x,y;\Xi) = F_{k+2,l} - 2F_{k+1,l+1} + F_{k,l+2} + \Xi F_{k,l}$.

[2] For $C_{k,l}$ we use $\arctan(\frac{Y}{Z}) = \frac{\pi}{2} - \arctan(\frac{Z}{Y})$ for $Y, Z > 0$.
For $C''_{k,l} = C^+_{k,l} + C^-_{k,l}$ use $\arctan(x) + \arctan(y) = \arctan\frac{x+y}{1-xy}$ $(0 \le xy \le 1)$ and $X, Y > 0$ according to Remark 3.13.

The x_3-integration uses

$$D_{k,l}(x,y;Y) = x^k y^l \frac{Y}{(x-y)^2 + Y^2},$$

$$E^+_{k,l}(x,y;X,Y) = \frac{x^k y^l}{2} X \ln \frac{\sqrt{(x-y)^2+\Theta} - Y}{\sqrt{(x-y)^2+\Theta} + Y}, \quad \Theta = X^2 + Y^2,$$

$$E^-_{k,l}(x,y;X,Y) = \frac{x^k y^l}{2} Y \ln \frac{\sqrt{(x-y)^2+\Theta} - X}{\sqrt{(x-y)^2+\Theta} + X} = E^+_{k,l}(x,y;Y,X). \tag{2.11}$$

Remark 2.1 *a) The functions $E^{\pm}_{k,l}$ are not independent of the previous ones but can be expressed via (3.3) as*

$$E^+_{k,l}(x,y;X,Y) = X\left[M_{k,l}(x,y;0,X) - M_{k,l}(x,y;Y,X)\right], \tag{2.12}$$

$$E^-_{k,l}(x,y;X,Y) = Y\left[M_{k,l}(x,y;0,Y) - M_{k,l}(x,y;X,Y)\right]. \tag{2.13}$$

b) Also $B_{k,l}$ can be expressed by means of $Q_{k,l}$ and $R^-_{k,l}$,

$$B_{k,l}(x,y;X,Y) = \frac{1}{Y}\left(Q_{k,l}(x,y;Y) - R^-_{k,l}(x,y;X,Y)\right). \tag{2.14}$$

c) The limits $R^+_{k,l}(x,y;0,Y) := \lim_{X\searrow 0} R^+_{k,l}(x,y;X,Y)$ for $Y>0$ will appear. Note that $R^+_{k,l}(x,y;0,Y) = x^k y^l \frac{\pi}{2}\operatorname{sign}(x-y)$ for $Y>0$. Similar functions appear in $G_{k,l}(x,y;0) = x^k y^l |x-y|$. Using

$$P^s_{k,l}(x,y) := x^k y^l \frac{\pi}{2}\operatorname{sign}(x-y),$$

we have

$$R^+_{k,l}(x,y;0,Y) = P^s_{k,l}(x,y).$$

We summarise that the result can be expressed by function evaluations of $G_{k,l}, L_{k,l}, M_{k,l}, P_{k,l}, Q_{k,l}, R^{\pm}_{k,l}$. The functions $A_{k,l}, B_{k,l}, C_{k,l}, C'_{k,l}, C''_{k,l}, C^{\pm}_{k,l}, D_{k,l}, E^{\pm}_{k,l}, P^s_{k,l}$ are used either for intermediate purpose or can be expressed via the functions of the first group.

The antiderivatives are denoted by the respective superscripts x or y. For example, $\mathcal{F}^x_{k,l}(x,y)$ satisfies $\frac{d}{dx}\mathcal{F}^x_{k,l}(x,y) = F_{k,l}(x,y)$ for $F_{k,l}$ from (2.2). The second antiderivative $\mathcal{F}^{xy}_{k,l}$ is defined by $\frac{d}{dy}\frac{d}{dx}\mathcal{F}^{xy}_{k,l} = F_{k,l}$.

3 Construction of Antiderivatives

3.1 First Integration (x_1)

In the first step, the antiderivative of $F_{k,l}$ with respect to x is to be determined.

Lemma 3.1 *$\mathcal{F}^x_{k,l}(x,y;\Xi)$ is a linear combination of*

$$\begin{array}{ll} \Xi^m G_{k',l'}(x,y;\Xi) & \text{for } 2m + k' + l' = k + l - 1, \\ \Xi^m L_{0,l'}(x,y;\Xi) & \text{for } 2m + l' = k + l, \end{array}$$

obtained via the recursion formulae (5.1), (5.2), (5.3).

Example 3.2 *$\mathcal{F}^x_{00} = L_{00}$ involves only the L-function. But $G_{k',l'}$ appears when $k \geq 1$, e.g., $\mathcal{F}^x_{1,0} = G_{00} + yL_{00}$. The factor Ξ appears for $k \geq 2$: $\mathcal{F}^x_{2,0} = \frac{1}{2}(3y+x)G_{00} + \left(y^2 - \frac{1}{2}\Xi\right)L_{00}$.*

3.2 Second Integration (y_1)

According to §3.1, $G_{k,l}$ and $L_{0,l}$ are to be integrated with respect to y. Using (5.9), $\mathcal{G}^y_{k,l}$ is expressed by $G_{k,l+1}$ and $\mathcal{F}^y_{k',l'}$ $(k'+l'\le k+l+2)$, while $\mathcal{L}^y_{0,l}$ yields $L_{0,l+1}$ and $\mathcal{F}^y_{k',l'}$ $(k'+l'\le l+1)$. Since the recursion formula for $\mathcal{F}^y_{k,l}$ is analog to $\mathcal{F}^x_{k,l}$, we obtain

Lemma 3.3 *a) $\mathcal{G}^y_{k,l}$ is a linear combination of $\Xi^m G_{k',l'}$ $(2m+k'+l'=k+l+1)$ and $\Xi^m L_{k',0}$ $(2m+k'=k+l+2)$ obtained by the combination of (5.9) and (5.4), (5.5), (5.6).*
b) $\mathcal{L}^y_{k,l}$ is a linear combination of $L_{k,l+1}$, $\Xi^m G_{k',l'}$ $(2m+k'+l'=k+l)$ and $\Xi^m L_{k',0}$ $(2m+k'=k+l+1)$ obtained by the combination of (5.7) and (5.4), (5.5), (5.6).

Applying both parts of Lemma 3.3 (with $k=0$ in Part b) to the result of Lemma 3.1, we obtain

Theorem 3.4 *The twofold antiderivative $\mathcal{F}^{xy}_{k,l}$ of $F_{k,l}$ with respect to x,y is a linear combination of*

$$\begin{array}{ll} \Xi^m G_{k',l'}(x,y;\Xi) & \text{for } 2m+k'+l'=k+l, \\ \Xi^m L_{k',0}(x,y;\Xi) & \text{for } 2m+k'=k+l+1, \\ \Xi^m L_{0,l'}(x,y;\Xi) & \text{for } 2m+l'=k+l+1. \end{array} \tag{3.1}$$

3.3 Example

The example of (1.3) with $k=l=0$ yields the twofold antiderivative

$$\mathcal{F}^{x_1y_1}_{00}(x_1,y_1;\Xi)=L_{01}-L_{10}+G_{00}=G_{00}(x_1,y_1;\Xi)-(x_1-y_1)\,L_{00}(x_1,y_1;\Xi).$$

Evaluation at the boundaries $x_1=0,1$ and $y_1=0,1$ results in

$$\begin{aligned} I_1(x_2,y_2,x_3,y_3) &:= \int_0^1\int_0^1 F_{00}(x_1,y_1;\Xi)\,dx_1dy_1=\mathcal{F}^{x_1y_1}_{00}|^1_{x_1=0}|^1_{y_1=0} \\ &= \ln\left(1+\sqrt{1+\Xi}\right)-\ln\left(-1+\sqrt{1+\Xi}\right)+2\sqrt{\Xi}-2\sqrt{1+\Xi}, \end{aligned} \tag{3.2}$$

where $\Xi=(x_2-y_2)^2+(x_3-y_3)^2$ contains the further variables (cf. (2.1)).

3.4 Interpretation as x_2,y_2-Functions

After the x_1,y_1-integration the variables x_1,y_1 are fixed by the integration bounds and thus become constants. Hence, $G_{k,l}=\mathit{const}*G_{00}$ and $L_{k,l}=\mathit{const}*L_{00}$.

Instead, we have to consider the x_2,y_2-variables hidden in $\Xi:=(x_2-y_2)^2+(x_3-y_3)^2$. Due to (2.1), we have $\sqrt{(x_1-y_1)^2+\Xi}=\sqrt{(x_2-y_2)^2+\Upsilon}$. Therefore, the function $G_{00}(x_1,y_1;\Xi)$ equals $G_{00}(x_2,y_2;\Upsilon)$. However, the function $L_{00}(x_1,y_1;\Xi)$ is not reproduced:

$$\begin{array}{rcll} G_{00}\left(x_1,y_1;Y^2+Z^2\right) &=& G_{00}\left(x_2,y_2;X^2+Z^2\right) & \text{with } X=x_1-y_1, Y=x_2-y_2, \\ L_{00}\left(x_1,y_1;Y^2+Z^2\right) &=& M_{00}(x_2,y_2;X,Z) & \text{(cf. (2.5) for } M_{k,l}). \end{array}$$

The function $M_{00}(x,y;X,Z)=\ln(X+\sqrt{(x-y)^2+X^2+Z^2})$ is analytic if $X>0$ and has a singularity only when $x=y$, $Z=0$, and $X\le 0$. This singularity is made more obvious by using $\ln(X+R)+\ln(-X+R)=\ln\left(R^2-X^2\right)$:

$$M_{k,l}(x,y;-X,Z)=-M_{k,l}(x,y;X,Z)+2M_{k,l}(x,y;0,Z). \tag{3.3}$$

The factors Ξ^m in (3.1) produce monomials of x_2 and y_2 of degree $2m$. This proves

Remark 3.5 *a) The functions to be integrated with respect to x_2,y_2 are $M_{k,l}(x_2,y_2;X,Z)$ and $G_{k,l}(x_2,y_2;\Upsilon)$ for various values of Υ and X. Because of (3.3) we may assume $X\ge 0$ for the second last argument of $M_{k,l}$.*
b) Starting with $F_{k,l}$ in §3.1, we arrive at $M_{k',l'}$ for $k'+l'\le k+l$ and $G_{k',l'}$ for $k'+l'\le k+l$.

Remark 3.6 *If the rectangle $R=\{(x_1,x_2): a_1'\le x_1\le b_1', a_2'\le x_2\le b_2'\}$ is replaced by a trapezium $\{(x_1,x_2): a_1'+c_2'x_2\le x_1\le b_1'+d_2'x_1, a_2'\le x_2\le b_2'\}$, the twofold antiderivative $\mathcal{F}^{xy}_{k,l}$ is to be evaluated an $x_1=a_1'+c_2'x_2, b_1'+d_2'x_1$. This gives rise to functions of x_2,y_2 different from $M_{k,l},G_{k,l}$ and therefore requires new considerations concerning the following integrations.*

3.5 Example

The result (3.2) can be rewritten as

$$2G_{00}\left(x_2,y_2;Z^2\right)-2G_{00}\left(x_2,y_2;1+Z^2\right)+M_{00}\left(x_2,y_2;1,Z\right)-M_{00}\left(x_2,y_2;-1,Z\right).$$

By (3.3), we obtain

$$2\left[G_{00}\left(x_2,y_2;Z^2\right)-G_{00}\left(x_2,y_2;1+Z^2\right)+M_{00}\left(x_2,y_2;1,Z\right)-M_{00}\left(x_2,y_2;0,Z\right)\right]. \tag{3.4}$$

Therefore, it remains to determine the x_2,y_2-antiderivatives of $M_{00}\left(x_2,y_2;X,Z\right)$ and $G_{00}\left(x_2,y_2;\Upsilon\right)$ for $\Upsilon=Z^2,1+Z^2$ and $X=0,1$.

3.6 Third Integration (x_2)

Now, x_2,y_2 are denoted shortly by x,y.

Similar to Part a) of Lemma 3.3, the antiderivative $\mathcal{G}_{k,l}^x$ of $G_{k,l}\left(x,y;\Upsilon\right)$ can be expressed by $G_{k+1,l}$ and $\mathcal{F}_{k',l'}^x$, while $\mathcal{F}_{k',l'}^x$ is discussed in Lemma 3.1.

Lemma 3.7 $\mathcal{G}_{k,l}^x\left(x,y;\Upsilon\right)$ *is a linear combination of*

$$\begin{array}{ll}\Upsilon^m G_{k',l'}\left(x,y;\Upsilon\right) & \text{for } 2m+k'+l'=k+l+1,\\ \Upsilon^m L_{0,l'}\left(x,y;\Upsilon\right) & \text{for } 2m+l'=k+l+2\end{array} \tag{3.5}$$

obtained by the combination of (5.8) and (5.1), (5.2), (5.3), where Ξ is replaced by Υ.

The antiderivative $\mathcal{M}_{k,l}^x$ of $M_{k,l}$ is expressed by $M_{k+1,l}$ and the antiderivatives of $\mathcal{A}_{k',l'}^x$ (cf. (5.16)). By the recursion formulae (5.10), (5.11), (5.12), one can replace $\mathcal{A}_{k,l}^x$ by $B_{0,l'},M_{0,l'},P_{k',l'},\mathcal{F}_{k',l'}^x$.

Lemma 3.8 *The antiderivative $\mathcal{M}_{k,l}^x\left(x,y;X,Z\right)$ of $M_{k,l}$ is a linear combination of $M_{k+1,l}$, $Z^{2n}M_{0,l'}$ $(2n+l'=k+l+1)$, $Z^{2n}B_{0,l'}$ $(2n+l'=k+l+2)$, $Z^{2n}P_{k',l'}$ $(2n+k'+l'=k+l+1)$, $Z^{2n}X\mathcal{F}_{k',l'}^x$ $(2n+k'+l'=k+l)$ obtained by (5.16), (5.10), (5.11), (5.12).*

Together with the recursion for $\mathcal{F}_{k,l}^x$ (cf. Lemma 3.1), one obtains

Theorem 3.9 *The x_2-integration of $G_{k,l}\left(x,y;\Upsilon\right)$ yielding (3.5) is discussed in Lemma 3.7, while $\mathcal{M}_{k,l}^x\left(x,y;X,Z\right)$ is a linear combination of*

$$\begin{array}{ll}Z^{2n}M_{k',l'}\left(x,y;X,Z\right) & \text{for } 2n+k'+l'=k+l+1,\\ Z^{2n}B_{0,l'}\left(x,y;X,Z\right) & \text{for } 2n+l'=k+l+2,\ n\geq 1,\\ Z^{2n}P_{k',l'}\left(x,y\right) & \text{for } 2n+k'+l'=k+l+1,\\ Z^{2n}X\Upsilon^m G_{k',l'}\left(x,y;\Upsilon\right) & \text{for } 2m+2n+k'+l'=k+l-1,\\ Z^{2n}X\Upsilon^m L_{0,l'}\left(x,y;\Upsilon\right) & \text{for } 2m+2n+l'=k+l,\end{array} \tag{3.6}$$

where[3] $\Upsilon:=X^2+Z^2$.

Proof. The inequality $n\geq 1$ for $Z^{2n}B_{0,l'}\left(x,y;X,Z\right)$ will be important. For its proof one has to check the recursions (5.10)-(5.12). The term $Z^2\mathcal{A}_{k-2,l}^x$ in (5.12) leads to $Z^{2n}B_{0,l'}$ with $n\geq 1$. Therefore omit this term from the recursion and note that the remaining recursions applied to the special difference $\mathcal{A}_{k+1,l+1}^x-\mathcal{A}_{k+2,l}^x$ appearing in (5.16) terminate for $k=1$ so that no $B_{0,l}$ is generated. ∎

3.7 Example

The functions appearing in (3.4) have the following antiderivatives ($\Upsilon:=X^2+Z^2$):

$$\begin{aligned}\mathcal{G}_{00}^x\left(x,y;\Upsilon\right)&=\frac{1}{2}\Upsilon L_{00}+\frac{1}{2}G_{10}-\frac{1}{2}G_{01}=\frac{1}{2}\left[\Upsilon L_{00}\left(x,y;\Upsilon\right)+(x-y)G_{00}\left(x,y;\Upsilon\right)\right],\\ \mathcal{M}_{00}^x\left(x,y;X,Z\right)&=Z^2B_{00}++XL_{00}M_{10}-M_{01}-x\\ &=Z^2B_{00}\left(x,y;X,Z\right)+XL_{00}\left(x,y;\Upsilon\right)+(x-y)\,M_{00}\left(x,y;X,Z\right)-x.\end{aligned}$$

[3] Note that $Z^{2n}X\Upsilon^m$ can be rewritten as a sum of terms of the form $Z^{2n'}X^{2m'+1}$ $(n'+m'=n+m)$.

3.8 Fourth Integration (y_2)

The y-integration of $G_{k,l}$ and $L_{0,l}$ (appearing in (3.5)) is already discussed in Lemma 3.3. The integration of $P_{k,l}$ yields $P_{k,l+1}/(l+1)$. Concerning $M_{k,l}$, the analogue of Lemma 3.8 is

Lemma 3.10 *The antiderivative $\mathcal{M}^y_{k,l}(x,y;X,Z)$ of $M_{k,l}$ is a linear combination of $M_{k,l+1}$, $Z^{2n}M_{k',0}$ $(2n+k'=k+l+1)$, $Z^{2n}B_{k',0}$ $(2n+k'=k+l+2)$, $Z^{2n}P_{k',l'}$ $(2n+k'+l'=k+l+1)$, $Z^{2n}X\mathcal{F}^y_{k',l'}$ $(2n+k'+l'=k+l)$ obtained by (5.17), (5.13), (5.14), (5.15). By means of (5.13), (5.14), (5.15), $Z^{2n}X\mathcal{F}^y_{k',l'}$ can be transferred into a linear combination of $Z^{2n}X\Upsilon^m G_{k',l'}(x,y;\Upsilon)$ $(2m+2n+k'+l'=k+l-1)$ and $Z^{2n}X\Upsilon^m L_{k',0}(x,y;\Upsilon)$ $(2m+2n+k'=k+l)$.*

Since X is already treated as constant, the factor X (e.g., in $Z^{2n}X\Upsilon^m G_{k',l'}$) can be omitted.
It remains to determine the antiderivatives $\mathcal{B}^y_{0,l}$ of $B_{0,l}$.

Lemma 3.11 *Due to (5.18), $\mathcal{B}^y_{0,l}$ can be expressed by $B_{0,l+1}$ and $\mathcal{A}^y_{0,l+1}$, while the latter term yields a sum of $Z^{2n}M_{k',0}$ $(2n+k'=l)$, $Z^{2n}P_{k',l'}$ $(2n+k'+l'=l)$, $Z^{2n}B_{k',0}$ $(2n+k'=l+1)$, $\Upsilon^m X Z^{2n} G_{k',l'}(x,y;\Upsilon)$ $(2m+2n+k'+l'=l-2)$ and $\Upsilon^m X Z^{2n} L_{k',0}(x,y;\Upsilon)$ $(2m+2n+k'=l-1)$.*

We summarise in

Theorem 3.12 *The twofold antiderivative $\mathcal{G}^{xy}_{k,l}(x,y;\Upsilon)$ is a linear combination of*

$$\begin{array}{ll} \Upsilon^m G_{k',l'}(x,y;\Upsilon) & \text{for } 2m+k'+l'=k+l+2,\ m\geq 0, \\ \Upsilon^m L_{0,l'}(x,y;\Upsilon) & \text{for } 2m+l'=k+l+3,\ m\geq 1, \\ \Upsilon^m L_{k',0}(x,y;\Upsilon) & \text{for } 2m+l'=k+l+3,\ m\geq 1, \end{array}$$

while $\mathcal{M}^{xy}_{k,l}(x,y;X,Z)$ is a linear combination of

$$\begin{array}{ll} Z^{2n}M_{k',l'}(x,y;X,Z) & \text{for } 2n+k'+l'=k+l+2, \\ Z^{2n}B_{k',l'}(x,y;X,Z) & \text{for } 2n+k'+l'=k+l+3,\ k'l'=0,\ n\geq 1, \\ Z^{2n}P_{k',l'}(x,y) & \text{for } 2n+k'+l'=k+l+2, \\ Z^{2n}X\Upsilon^m G_{k',l'}(x,y;\Upsilon) & \text{for } 2m+2n+k'+l'=k+l, \\ Z^{2n}X\Upsilon^m L_{k',l'}(x,y;\Upsilon) & \text{for } 2m+2n+k'+l'=k+l+1,\ k'l'=0. \end{array}$$

3.9 Example

Due to (3.4), the twofold antiderivatives $\mathcal{G}^{xy}_{00}$ and $\mathcal{M}^{xy}_{00}$ are required. The result is[4]

$$\begin{aligned} \mathcal{G}^{xy}_{00}(x,y;\Upsilon) &= -\frac{1}{2}\Upsilon(x-y)L_{00}(x,y;\Upsilon)+\frac{1}{6}\left(2\Upsilon-(x-y)^2\right)G_{00}(x,y;\Upsilon), \\ \mathcal{M}^{xy}_{00}(x,y;X,Z) &= -(x-y)Z^2B_{00}(x,y;X,Z)+\frac{1}{2}XG_{00}(x,y;\Upsilon)-(x-y)XL_{00}(x,y;\Upsilon) \\ &\quad +\frac{1}{2}\left(Z^2-(x-y)^2\right)M_{00}(x,y;X,Z)+\frac{1}{4}y^2-\frac{3}{2}xy, \end{aligned}$$

where Z^2 is introduced via $X^2+Z^2=\Upsilon$. Inserting the different arguments for Υ and X appearing in (3.4), we obtain finally

$$J_2\left(x_2,y_2;Z^2\right)=\left\{\begin{array}{lll} 2(x_2-y_2)Z^2B_{00}(x_2,y_2;0,Z) & - & 2(x_2-y_2)Z^2B_{00}(x_2,y_2;1,Z) \\ +\frac{2Z^2-(x_2-y_2)^2}{3}G_{00}\left(x_2,y_2;Z^2\right) & + & \frac{1-2Z^2+(x_2-y_2)^2}{3}G_{00}\left(x_2,y_2;1+Z^2\right) \\ -Z^2(x_2-y_2)L_{00}\left(x_2,y_2;Z^2\right) & + & \left(Z^2-1\right)(x_2-y_2)L_{00}\left(x_2,y_2;1+Z^2\right) \\ -\left(Z^2-(x_2-y_2)^2\right)M_{00}(x_2,y_2;0,Z) & + & \left(Z^2-(x_2-y_2)^2\right)M_{00}(x_2,y_2;1,Z). \end{array}\right. \tag{3.7}$$

[4]The polynomial $\frac{1}{4}y^2-\frac{3}{2}xy$ can be replaced by $\frac{3}{4}(x-y)^2$, since y^2 and x^2 terms do not matter for the twofold antiderivative. In the later differences, the polynomials will disappear in any way.

3.10 Interpretation as x_3, y_3-Functions

All functions listed in (3.5) and (3.6) are to be evaluated at certain x_2, y_2-values (written above as x, y). Hence, x_2, y_2 as well as $Y = x_2 - y_2$ are considered as constants. The x_3, y_3-variables appear in $Z = x_3 - y_3$ and $\Upsilon = X^2 + Z^2$. The factors Z^{2n} are polynomials in x_3, y_3 of degree $2n$. Similarly, Υ^m is a polynomial of degree $2m$.

In the following the functions $G_{k,l}, \ldots$ are considered as functions of the variables x_3, y_3. Since the indices k, l refer to $x_2^k y_2^l$, which is now a constant after the evaluation, it suffices to discuss $G_{00}, \ldots$. We have $G_{00}(x_2, y_2; \Upsilon) = \sqrt{(x_2 - y_2)^2 + \Upsilon} = \sqrt{(x_3 - y_3)^2 + \Theta}$, where $\Theta = X^2 + Y^2 = (x_1 - y_1)^2 + (x_2 - y_2)^2$ is a fixed constant. The new function of the variables x_3, y_3 is again G_{00}, but now with the arguments $G_{00}(x_3, y_3; \Theta)$. The complete list is

$$\begin{array}{lcll} G_{00}\left(x_2, y_2; X^2 + Z^2\right) & = & G_{00}\left(x_3, y_3; X^2 + Y^2\right), & \text{with } Y = x_2 - y_2, Z = x_3 - y_3, \\ L_{00}\left(x_2, y_2; X^2 + Z^2\right) & = & M_{00}\left(x_3, y_3; Y, X\right) & \\ M_{00}\left(x_2, y_2; X, Z\right) & = & M_{00}\left(x_3, y_3; X, Y\right) & \text{(cf. (2.5))}, \\ Z^2 B_{00}\left(x_2, y_2; X, Z\right) & = & C_{00}\left(x_3, y_3; X, Y\right) & \text{(cf. (2.7))}, \\ 1 & = & P_{00}\left(x_3, y_3\right). & \end{array}$$

The equality $Z^2 B_{00} = C_{00}$ needs some care as discussed in

Remark 3.13 *a) Due to Remark 3.5, we have $X \geq 0$. Let $Y = x_2 - y_2$ be a fixed value. Applying*

$$B_{00}\left(x_2, y_2; X, Z\right) = -B_{00}\left(y_2, x_2; X, Z\right) = -B_{00}\left(-x_2, -y_2; X, Z\right)$$

for $Y < 0$, we can ensure $Y \geq 0$. Since $Y = 0$ implies $B_{00}\left(x_2, x_2; X, Z\right) = 0$, we may even assume $Y > 0$.

b) The case $X = 0, Y > 0$ can be considered as the limit case $X \searrow 0$ resulting in $C_{00} = C_{00}^{+} + C_{00}^{-} - C_{00}'$ with $C_{00}^{+}\left(x_3, y_3; 0, Y\right) := \frac{\pi}{2}\left|x_3 - y_3\right|$ and $C_{00}^{-}\left(x_3, y_3; 0, Y\right) = 0$.

c) Under the condition $X, Y > 0$, the equality $Z^2 B_{00}\left(x_2, y_2; X, Z\right) = C_{00}\left(x_3, y_3; X, Y\right)$ holds.

Proof. c) Assume $X, Y > 0$. Note that $B_{00}\left(x_2, y_2; X, Z\right) = \frac{1}{Z}\left(\arctan\frac{Y}{Z} - \arctan\frac{XY}{Z\sqrt{Z^2+\Theta}}\right)$ $(Y = x_2 - y_2)$ is an even function with respect to Z. Choose $Z > 0$. Then $X, Y, Z > 0$ implies $\arctan\frac{Y}{Z} = \frac{\pi}{2} - \arctan\frac{Z}{Y}$ and $\arctan\frac{XY}{Z\sqrt{Z^2+\Theta}} = \frac{\pi}{2} - \arctan\frac{Z\sqrt{Z^2+\Theta}}{XY}$, which results in $Z^2 B_{00}\left(x_2, y_2; X, Z\right) = Z\left(\arctan\frac{Z\sqrt{Z^2+\Theta}}{XY} - \arctan\frac{Z}{Y}\right)$ $= C_{00}\left(x_3, y_3; X, Y\right)$ $(Z = x_3 - y_3)$. Since the right-hand side is again an even function in $Z = x_3 - y_3$, the equality $Z^2 B_{00} = C_{00}$ holds for all x_3, y_3. ■

3.11 Example

The function $J_2\left(x_2, y_2; Z^2\right) = J_2\left(x_2, y_2; (x_3 - y_3)^2\right)$ from (3.7) is to be evaluated at the boundaries $0, 1$ of the cubes B', B'' (cf. (1.3)). Since G_{00} as well as L_{00}, M_{00}, B_{00} depend only on $x - y$, we rewrite $G_{00}(x, y; \ldots)$ as $G_{00}(x - y; \ldots)$. Then

$$\begin{aligned} & J_2\left(x_2, y_2; Z^2\right)\Big|_{x_2=0}^{1}\Big|_{y_2=0}^{1} = J_2\left(1, 1; Z^2\right) + J_2\left(0, 0; Z^2\right) - J_2\left(1, 0; Z^2\right) - J_2\left(0, 1; Z^2\right) \\ & = -4Z^2 B_{00}\left(1; 0, Z\right) + 4Z^2 B_{00}\left(1; 1, Z\right) \\ & + \frac{4Z^2}{3} G_{00}\left(0; Z^2\right) + \frac{2 - 4Z^2}{3} G_{00}\left(0; 1 + Z^2\right) + \frac{2 - 4Z^2}{3} G_{00}\left(1; Z^2\right) + \frac{4Z^2 - 4}{3} G_{00}\left(1; 1 + Z^2\right) \\ & - 2Z^2 L_{00}\left(0; Z^2\right) + 2\left(Z^2 - 1\right) L_{00}\left(0; 1 + Z^2\right) + 2Z^2 L_{00}\left(1; Z^2\right) - 2\left(Z^2 - 1\right) L_{00}\left(1; 1 + Z^2\right) \\ & - 2Z^2 M_{00}\left(0; 0, Z\right) + 2Z^2 M_{00}\left(0; 1, Z\right) + 2\left(Z^2 - 1\right) M_{00}\left(1; 0, Z\right) - 2\left(Z^2 - 1\right) M_{00}\left(1; 1, Z\right). \end{aligned}$$

Its expression as function of x_3, y_3 is

$$\begin{aligned} I_2(x, y) = {} & 8C_{00}^{+}(x, y; 1, 1) + \frac{4}{3}(x - y)^2 G_{00}(x, y; 0) + \left(\frac{4}{3} - \frac{8}{3}(x - y)^2\right) G_{00}(x, y; 1) \\ & + \left(-\frac{4}{3} + \frac{4}{3}(x - y)^2\right) G_{00}(x, y; 2) - 4(x - y)^2 M_{00}(x, y; 0, 0) + 4(x - y)^2 M_{00}(x, y; 1, 0) \\ & + \left(-4 + 4(x - y)^2\right) M_{00}(x, y; 0, 1) + \left(4 - 4(x - y)^2\right) M_{00}(x, y; 1, 1) - 2\pi\left|x - y\right|. \end{aligned} \tag{3.8}$$

3.12 Fifth Integration (x_3)

Now, x_3, y_3 are denoted shortly by x, y.

The antiderivatives $\mathcal{G}_{k,l}^x$ and $\mathcal{M}_{k,l}^x$ are known from above. The x-integration of $L_{k,l}$ is similar to the y-integration discussed in Lemma 3.3.

The only new function to be considered is $C_{k,l}(x,y;X,Y)$. For its integration we split $C_{k,l}$ into the terms $C'_{k,l}$ and $C^{\pm}_{k,l}$ defined in (2.8) and (2.9), respectively, and introduce auxiliary functions $D_{k,l}$, $Q_{k,l}$, $R^{\pm}_{k,l}$, $E^{\pm}_{k,l}$ (cf. (2.10)-(2.11)). The final result is then given by Lemma 3.16.

Lemma 3.14 *The antiderivative $\mathcal{D}^x_{k,l}(x,y;Y)$ of $D_{k,l}(x,y;Y) = x^k y^l \frac{Y}{(x-y)^2+Y^2}$ can be determined by the recursion (5.19), (5.20), (5.21) which yields a linear combination of*

$$\begin{array}{ll} Y^{2m}Q_{0,l'} & \text{for } 2m+l'=k+l, \\ Y^{2m+1}M_{0,l'}(x,y;0,Y) & \text{for } 2m+1+l'=k+l, \\ Y^{2m+1}P_{k',l'}(x,y) & \text{for } 2m+1+k'+l'=k+l. \end{array} \tag{3.9}$$

Note that the formulae make sense only if $Y\neq 0$; otherwise, $D_{k,l}(x,y;0)\equiv 0$ implies $\mathcal{D}^x_{k,l}(x,y;0)\equiv 0$.

Lemma 3.15 *The x-antiderivatives of $R^+_{k,l}(x,y;X,Y), E^+_{k,l}(x,y;X,Y)$ can be determined by the combined recursions (5.23)-(5.26). $\mathcal{R}^{+x}_{k,l}$ is a linear combination of*

$$\begin{array}{ll} X^{2m}R^+_{k',l'}(x,y;X,Y) & \text{for } 2m+k'+l'=k+l+1, \\ X^{2m}E^+_{k',l'}(x,y;X,Y) & \text{for } 2m+k'+l'=k+l, \\ X^{2m+1}Y\Theta^n G_{k',l'}(x,y;\Theta) & \text{for } 2m+2n+k'+l'=k+l-2,\ \Theta=X^2+Y^2, \\ X^{2m+1}Y\Theta^n L_{0,l'}(x,y;\Theta) & \text{for } 2m+2n+l'=k+l-1, \end{array} \tag{3.10}$$

while $\mathcal{E}^{+x}_{k,l}$ is a linear combination of

$$\begin{array}{ll} X^{2m}R^+_{k',l'}(x,y;X,Y) & \text{for } 2m+k'+l'=k+l,\ m\geq 1, \\ X^{2m}E^+_{k',l'}(x,y;X,Y) & \text{for } 2m+k'+l'=k+l+1, \\ X^{2m+1}Y\Theta^n G_{k',l'}(x,y;\Theta) & \text{for } 2m+2n+k'+l'=k+l-1,\ \Theta=X^2+Y^2, \\ X^{2m+1}Y\Theta^n L_{0,l'}(x,y;\Theta) & \text{for } 2m+2n+l'=k+l. \end{array}$$

In the case of $R^-_{k,l}(x,y;X,Y)$ and $E^-_{k,l}(x,y;X,Y)$, one has to interchange X and Y. Due to (2.12), (2.13), $E^+_{k',l'}$ in (3.10) can be replaced by $M_{k',l'}$.

The antiderivatives $\mathcal{D}^x_{k,l}$ and $\mathcal{R}^{+x}_{k,l}, \mathcal{E}^{+x}_{k,l}$ are needed to integrate $C_{k,l} = C^+_{k,l} + C^-_{k,l} - C'_{k,l}$.

Lemma 3.16 *a) The antiderivative $\mathcal{C}'^x_{k,l}(x,y;Y)$ of $C'_{k,l}$ can be obtained by the recursion formulae (5.28), (5.28). $\mathcal{C}'^x_{k,l}$ is a linear combination of $Q_{k',l'}$ $(k'+l'=k+l)$ and the functions in (3.9).*

b) The antiderivative $\mathcal{C}^{+x}_{k,l}(x,y;X,Y)$ of $C^+_{k,l}$ can be obtained by the recursion formulae (5.23)-(5.26) and is a linear combination of the functions from (3.10) and with $k+l$ replaced by $k+l+1$. Similarly for $\mathcal{C}^{+y}_{k,l}$.

c) Concerning the limit case ($X\searrow 0$) of $C^+_{00}(x,y;0,Y) = \frac{\pi}{2}|x-y|$ from Remark 3.13b, we remark that the x-antiderivative of $x^k\operatorname{sign}(x-y)$ is $\left(x^{k+1}-y^{k+1}\right)\operatorname{sign}(x-y)/(k+1)$.

3.13 Sixth Integration (y_3)

The two-fold antiderivatives $\mathcal{G}^{xy}_{k,l}$ and $\mathcal{M}^{xy}_{k,l}$ are known from above. The y-integration of $C_{k,l} = C^+_{k,l} + C^-_{k,l} - C'_{k,l}$ requires the y-antiderivatives of $Q_{k,l}, M_{0,l}(x,y;0,Y), P_{k,l}, T^{\pm}_{0,l}, R^{\pm}_{k,l}, E^{\pm}_{k,l}, G_{k,l}, L_{0,l}$. Only the recursion (5.22) for $Q_{k,l}$ is new. In the other cases the y-integration is already discussed or similar to the x-integration.

3.14 Example

The second antiderivative of (3.8) is the following function of $x = x_3$ and $y = y_3$:

$$
\begin{aligned}
J_3(x,y) = & -\frac{1}{15}(x-y)^4 G_{00}(x,y;0) + \left(\frac{2}{15} - \frac{2}{5}(x-y)^2 + \frac{2}{15}(x-y)^4\right) G_{00}(x,y;1) \\
& + \left(\frac{1}{15} + \frac{2}{5}(x-y)^2 - \frac{1}{15}(x-y)^4\right) G_{00}(x,y;2) - \frac{x-y}{3} L_{00}(x,y;1) - \frac{2}{3}(x-y) L_{00}(x,y;2) \\
& + \frac{1}{3}(x-y)^4 M_{00}(x,y;0,0) - \frac{1}{3}(x-y)^4 M_{00}(x,y;1,0) \\
& + \left(-\frac{1}{3} + 2(x-y)^2 - \frac{1}{3}(x-y)^4\right) M_{00}(x,y;0,1) + \left(\frac{1}{3} - 2(x-y)^2 + \frac{1}{3}(x-y)^4\right) M_{00}(x,y;1,1) \\
& + \frac{\pi}{3}(x-y)^2 |x-y| + \left(\frac{4}{3} - \frac{4}{3}(x-y)^2\right)(x-y) R_{00}^{+}(x,y;1,1).
\end{aligned} \tag{3.11}
$$

The integral $I_3 = \int_1^2 \left(\int_0^1 I_2(x,y)\,dy\right) dx = J_3(2,1) - J_3(2,0) - J_3(1,1) + J_3(1,0)$ corresponds to (1.3) and equals $0.9808851836\ldots$, which is the numerical evaluation of

$$
\begin{aligned}
I_{face} := I([0,1]^2 \times [1,2], [0,1]^3) = & \frac{28}{15} - 2\pi + 8\arctan\sqrt{\frac{2}{3}} - \frac{1}{3}\sqrt{2} + \frac{4}{5}\sqrt{3} - \frac{2}{3}\sqrt{5} - \frac{3}{5}\sqrt{6} - 4\ln 2 - \frac{7}{6}\ln 5 \\
& - \frac{5}{3}\ln\left(1+\sqrt{2}\right) - 4\ln\left(1+\sqrt{3}\right) + \frac{16}{3}\ln\left(1+\sqrt{5}\right) + \frac{7}{3}\ln\left(1+\sqrt{6}\right) + \frac{2}{3}\ln\left(2+\sqrt{5}\right) + \frac{4}{3}\ln\left(2+\sqrt{6}\right).
\end{aligned}
$$

As a verification we give the numerical result of the Gauß quadrature rule with 12 quadrature points in each of the three dimensions: $0.9810823\ldots$. Note that this quadrature is of limited accuracy because of the singularity along the common face of $[0,1]^2 \times [1,2]$ and $[0,1]^3$.

Similarly, the integral for two unit cubes intersecting only in one edge is

$$
\begin{aligned}
& I_{edge} := I([0,1] \times [1,2]^2, [0,1]^3) = 0.708\,495\,126\,86\ldots = \\
& -\frac{88}{15} + 2\pi - 16\arctan\sqrt{\frac{2}{3}} + 4\arctan\frac{4}{3} + \frac{4}{3}\sqrt{2} - \frac{4}{5}\sqrt{3} + \sqrt{5} + \frac{6}{5}\sqrt{6} + 10\ln 2 + \frac{7}{2}\ln 5 \\
& + \frac{20}{3}\ln\left(1+\sqrt{2}\right) + 4\ln\left(1+\sqrt{3}\right) - 8\ln\left(1+\sqrt{5}\right) - \frac{14}{3}\ln\left(1+\sqrt{6}\right) - \ln\left(2+\sqrt{5}\right) - \frac{8}{3}\ln\left(2+\sqrt{6}\right).
\end{aligned}
$$

Here, the Gauß quadrature leads to $0.708\,495\,88\ldots$.

Two unit cubes intersecting in one corner yield

$$
\begin{aligned}
& I_{corner} := I([1,2]^3, [0,1]^3) = 0.578\,797\,001\,778\ldots = \\
& + \frac{66}{5} - 4\pi + 24\arctan\sqrt{\frac{2}{3}} - 16\arctan\frac{4}{3} + 8\arctan 3 - \frac{9}{5}\sqrt{2} - \frac{12}{5}\sqrt{3} - \sqrt{5} - \frac{9}{5}\sqrt{6} - 24\ln 2 - 7\ln 5 \\
& - 9\ln\left(1+\sqrt{2}\right) + 12\ln\left(1+\sqrt{3}\right) + 8\ln\left(1+\sqrt{5}\right) + 7\ln\left(1+\sqrt{6}\right) + \ln\left(2+\sqrt{5}\right) + 4\ln\left(2+\sqrt{6}\right),
\end{aligned}
$$

which is to be compared with the Gauß result $0.578\,797\,001\,808\ldots$.

Two identical cube lead to

$$
\begin{aligned}
& I_{id} := I([0,1]^3, [0,1]^3) = 1.882312644\ldots = \\
& + \frac{2}{5} - \frac{2}{3}\pi + \frac{2}{5}\sqrt{2} - \frac{4}{5}\sqrt{3} - 2\ln 2 + 2\ln\left(1+\sqrt{2}\right) + 4\ln\left(1+\sqrt{3}\right).
\end{aligned}
$$

In this case the singularity is too strong to use the simple Gauß quadrature, but the result satisfies the following

Remark 3.17 *The identity* $I_{id} = I_{face} + I_{edge} + \frac{1}{3} I_{corner}$ *holds.*

Proof. Divide the integral $I([0,2]^3, [0,2]^3) = 4I_{id}$ into 64 integrals over unit cubes. ∎

3.15 Stabilisation

The evaluation of the symbolic results like in (3.11) needs some care when $x-y$ becomes large. The reason is that the final result I_3 must decay as $1/r$ with $r=|x-y|$ while some of the summands increase polynomially. Either one uses a high accuracy for the evaluation of the functions or tries to reduce cancellation, e.g., by using

$$\sqrt{X}-\sqrt{Y}=\frac{X-Y}{\sqrt{X}+\sqrt{Y}},\qquad \ln\left(a+\sqrt{b^2+R^2}\right)=\ln(R)+\ln\left(\frac{a}{R}+\sqrt{\frac{b^2}{R^2}+1}\right),$$

$$\arctan\frac{\rho r}{\sqrt{r^2+R^2}}=\arctan\rho-\arctan\frac{\rho R^2}{\left(\sqrt{r^2+R^2}+\rho^2 r\right)\left(r+\sqrt{r^2+R^2}\right)}\qquad \text{for large } r\ge 0 \text{ and } \rho\ge 0$$

for differences of G_{00}, L_{00}, M_{00} and $R_{00}^{\pm}$ functions. To illustrate the problem, we remark that the result for $B'=[0,100]\times[0,1]\times[0,1]$ and $B''=[0,1]\times[0,100]\times[0,1]$ and $\nu_i=\mu_i=0$ equals $181.4\ldots$ It is a sum $\sum a_i$ of 51 terms with different signs. The sum $\sum|a_i|=8.3_{10}+10$ yields the condition number[5] $4.6_{10}{+}8$ so that only 7-8 digits of the result are accurate. While the complete result can be found in §6.10, we show only a group of 6 terms involving square roots of similar size:

$$-\frac{32019867}{5}*\sqrt{9801}+\frac{192060398}{15}*\sqrt{9802}-\frac{96000794}{15}*\sqrt{9803}$$
$$+\frac{20000000}{3}*\sqrt{10000}-\frac{199940002}{15}*\sqrt{10001}+\frac{33313333}{5}*\sqrt{10002}.$$

Their sum is $-0.41667\ldots$, whereas the sum of absolute terms equals $5.2_{10}{+}9$ indicating a loss of 10 digits. Since the sum of the rather large coefficients vanishes exactly, a simple remedy is the use of $\sqrt{10000+\delta}=100+w(\delta)$ with $w(\delta)=\frac{\delta}{\sqrt{10000+\delta}+100}$ for $\delta\in\{-199,-198,-197,0,1,2\}$. The condition number of the resulting sum $-\frac{32019867}{5}*w(-199)+\ldots$ is reduced to $2.5_{10}{+}7$.

3.16 Symbolic Computation

The type of quantities to be treated are sums of linear combinations like $\sum_{k,l}a_{k,l}^{G}G_{k,l}$, $\sum_{k,l}a_{k,l}^{M}M_{k,l}$ etc. The latter sums can be written as $\left(\sum_{k,l}a_{k,l}^{G}(\Xi)\,x^k y^l\right)G_{00}(x,y;\Xi)$, $\left(\sum_{k,l}a_{k,l}^{M}(Z^2)\,x^k y^l\right)M_{00}(x,y;X,Z)$ etc. The first factor is a polynomial in x,y with coefficients being polynomials in a further parameter. The following steps have to be performed:

1. The starting function is $x_1^{\nu_1}y_1^{\mu_1}F_{00}(x_1,y_1;\Xi)=F_{\nu_1,\mu_1}(x_1,y_1;\Xi)$, which may be generalised to a polynomial $f(x_1,y_1;\Xi):=\sum_{k,l}a_{k,l}^{F}F_{k,l}(x_1,y_1;\Xi)$.

   a) Apply the recursions (5.1)-(5.3) to obtain $g=\sum_{k,l}a_{k,l}^{G}G_{k,l}$ and $\ell=\sum_{k,l}a_{k,l}^{L}L_{k,l}$ with the arguments $(x_1,y_1;\Xi)$. Note that the coefficients are polynomials in Ξ.

   b) Given g,ℓ, apply the recursions (5.9), (5.7) and (5.4)-(5.6) to obtain new g,ℓ. Then $J_0(x_1,y_1;\Xi):=g+\ell$ is the twofold antiderivative of f.

   c) Evaluate $I_1(\Xi):=J_0(a_1',a_1'';\Xi)-J_0(a_1',b_1'';\Xi)-J_0(b_1',a_1'';\Xi)+J_0(b_1',b_1'';\Xi)$ at the integral bounds (cf. (1.2)).

   d) Interpret $I_1(\Xi)=I_1(x_2,y_2;Z)$ as a function of x_2,y_2 (cf. §3.4).

2. The result of Step 1d is $I_1(x_2,y_2;Z)$, which is a sum of g_i and m_i, where

   $$g_i(x_2,y_2;Z)=\sum_{k,l}a_{k,l}^{G,i}G_{k,l}(x_2,y_2;X_i^2+Z^2),\quad m_i(x_2,y_2;Z)=\sum_{k,l}a_{k,l}^{M,i}M_{k,l}(x_2,y_2;X_i,Z)$$

   for various X_i. The coefficients $a_{k,l}^{G,i}$ can be organised as polynomials in $X_i^2+Z^2$, while $a_{k,l}^{M,i}$ may be written as polynomial in Z^2.

[5]The condition number of a sum is defined by $\sum|a_i|\,/\,|\sum a_i|$.

a) Multiply $I_1(x_2, y_2; Z)$ by $x_2^{\nu_2} y_2^{\mu_2}$ from (1.1).

b) Apply the recursions for $G_{k,l}$,$M_{k,l}$ to obtain the x-antiderivative as sum of new m_i, b_i, p, g, ℓ corresponding to $M_{k,l}(x_2, y_2; X_i, Z)$, $B_{k,l}(x_2, y_2; X_i, Z)$, $P_{k,l}(x_2, y_2)$, $G_{k,l}(x_2, y_2; X_i^2 + Z^2)$, and $L_{k,l}(x_2, y_2; X_i^2 + Z^2)$. Note that $X = X_i$ in recursion (5.12) is a constant.

c) Apply the recursions for $G_{k,l}, L_{k,l}, M_{k,l}, B_{k,l}, P_{k,l}$ to obtain the y-antiderivative as sum of new m_i, b_i, p, g_i, ℓ_i. The result is denoted by $J_1(x_2, y_2; Z)$.

d) Evaluate $I_2(Z) := J_1(a_2', a_2''; Z) - J_1(a_2', b_2''; Z) - J_1(b_2', a_2''; Z) + J_1(b_2', b_2''; Z)$.

e) Interpret $I_2(Z)$ as function of x_3, y_3 (cf. §3.10).

3. The result of Step 2e is $I_2(x_3, y_3)$, which is a sum of $g_i, m_i, c_i', c_i^{\pm}$, where, e.g.,

$$c_i^+(x_2, y_2; Z) = \sum_{k,l} a_{k,l}^{C^+,i} C_{k,l}^+(x_3, y_3; X_i, Y_i)$$

for certain X_i, Y_i. The coefficients $a_{k,l}^{C^+,i}$ are constants.

a) Multiply $I_2(x_3, y_3)$ by $x_3^{\nu_3} y_3^{\mu_3}$ from (1.1).

b) Apply the recursions to obtain the twofold antiderivative $J_2(x_3, y_3)$ of $I_2(x_3, y_3)$.

c) Evaluate the final value of (1.1) by $I(B', B'') = J_2(a_3', a_3'') - J_2(a_3', b_3'') - J_2(b_3', a_3'') + J_2(b_3', b_3'')$.

A program realising these steps is described in §6.

4 Collocation

The integral

$$\iiint_B \frac{x_1^{\nu_1} x_2^{\nu_2} x_3^{\nu_3}}{\sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2}^2} dx_1 dx_2 dx_3 \qquad \text{for } \mathbf{y} = (y_1, y_2, y_3) \in \mathbb{R}^3 \tag{4.1}$$

with $B = \prod_{i=1}^3 [a_i, b_i]$ appears, e.g., in the collocation method and can be treated similarly.

After the first integration (see §3.1), we have to insert the x_1-values from the integral bounds and the y_1-value fixed in (4.1) into the antiderivative. A comparison of Lemma 3.1 with Theorem 3.4 shows that the arising expressions are of the same form as those obtained previously from the twofold antiderivative. Similar statements hold for the x_2- and x_3-integration.

5 Recursion Formulae

5.1 F

The x- and y-integration of $F_{k,l}$ yields $\mathcal{F}_{k,l}^x \to G_{k',l'}, L_{0,l'}$ and $\mathcal{F}_{k,l}^y \to G_{k',l'}, L_{k',0}$ (cf. Lemma 3.1):

$$\mathcal{F}_{0,l}^x(x, y; \Xi) = L_{0,l}(x, y; \Xi), \tag{5.1}$$

$$\mathcal{F}_{1,l}^x(x, y; \Xi) = G_{0,l}(x, y; \Xi) + L_{0,l+1}(x, y; \Xi), \tag{5.2}$$

$$\mathcal{F}_{k,l}^x(x, y; \Xi) = \frac{G_{k-1,l} + (2k-1)\mathcal{F}_{k-1,l+1}^x - (k-1)\mathcal{F}_{k-2,l+2}^x - (k-1)\Xi\mathcal{F}_{k-2,l}^x}{k} \quad \text{for } k \geq 2. \tag{5.3}$$

Proof. $\frac{d}{dx} G_{k-1,l} = x^{k-2} y^l \frac{k(x-y)^2 + (k-1)\Xi + y(x-y)}{\sqrt{(x-y)^2 + \Xi}} = kF_{k,l} - (2k-1) F_{k-1,l+1} + (k-1) F_{k-2,l+2} + (k-1)\Xi F_{k-2,l}$ proves (5.3) for $\mathcal{F}_{k,l}^x$, while (5.1) and (5.2) are trivial. ■

$$\mathcal{F}_{k,0}^y(x, y; \Xi) = -L_{k,0}(x, y; \Xi), \tag{5.4}$$

$$\mathcal{F}_{k,1}^y(x, y; \Xi) = G_{k,0}(x, y; \Xi) - L_{k+1,0}(x, y; \Xi), \tag{5.5}$$

$$\mathcal{F}_{k,l}^y(x, y; \Xi) = \frac{G_{k,l-1} + (2l-1)\mathcal{F}_{k+1,l-1}^y - (l-1)\mathcal{F}_{k+2,l-2}^y - (l-1)\Xi\mathcal{F}_{k,l-2}^y}{l} \quad \text{for } l \geq 2. \tag{5.6}$$

Proof. For $\mathcal{F}_{k,l}^y$ use $\frac{d}{dy} G_{k,l-1} = lF_{k,l} - (2l-1) F_{k+1,l-1} - (l-1) F_{k+2,l-2} + (l-1)\Xi F_{k,l-2}$. ■

5.2 L

Integration of $\frac{d}{dx}L_{k+1,l} = (k+1)\,L_{k,l} + F_{k+1,l}$ and $\frac{d}{dy}L_{k,l+1} = (l+1)\,L_{k,l} - F_{k,l+1}$ yields the following expressions for the x- and y-antiderivatives $\mathcal{L}^x_{k,l}, \mathcal{L}^y_{k,l}$ of $L_{k,l}$ (cf. Lemma 3.3):

$$
\begin{aligned}
\mathcal{L}^x_{k,l}\,(x,y;\Xi) &= \frac{L_{k+1,l}\,(x,y;\Xi) - \mathcal{F}^x_{k+1,l}\,(x,y;\Xi)}{k+1}, \\
\mathcal{L}^y_{k,l}\,(x,y;\Xi) &= \frac{L_{k,l+1}\,(x,y;\Xi) + \mathcal{F}^y_{k,l+1}\,(x,y;\Xi)}{l+1}.
\end{aligned} \tag{5.7}
$$

5.3 G

For $\mathcal{G}^x_{k,l}$ use $\frac{d}{dx}G_{k+1,l} = (k+1)\,G_{k,l} + F_{k+2,l} - F_{k+1,l+1}$, while $\frac{d}{dy}G_{k,l+1} = (l+1)\,G_{k,l} + F_{k,l+2} - F_{k+1,l+1}$ proves the recursion for $\mathcal{G}^y_{k,l}$ (cf. Lemmata 3.7, 3.3):

$$
\mathcal{G}^x_{k,l}\,(x,y;\Xi) = \frac{G_{k+1,l}\,(x,y;\Xi) - \mathcal{F}^x_{k+2,l}\,(x,y;\Xi) + \mathcal{F}^x_{k+1,l+1}\,(x,y;\Xi)}{k+1}, \tag{5.8}
$$

$$
\mathcal{G}^y_{k,l}\,(x,y;\Xi) = \frac{G_{k,l+1}\,(x,y;\Xi) - \mathcal{F}^y_{k,l+2}\,(x,y;\Xi) + \mathcal{F}^y_{k+1,l+1}\,(x,y;\Xi)}{l+1}. \tag{5.9}
$$

5.4 A

The auxiliary function $A_{k,l}$ will be needed in the next subsections.

The x- and y-integration of $A_{k,l}$ yields $\mathcal{A}^x_{kl} \to B_{0,l'}, M_{0,l'}, P_{k',l'}, \mathcal{F}^x_{k',l'}$:

$$
\mathcal{A}^x_{0,l}\,(x,y;X,Z) = B_{0,l}\,(x,y;X,Z)\,, \tag{5.10}
$$

$$
\mathcal{A}^x_{1,l}\,(x,y;X,Z) = \mathcal{A}^x_{0,l+1}\,(x,y;X,Z) + M_{0,l}\,(x,y;X,Z)\,, \tag{5.11}
$$

$$
\mathcal{A}^x_{k,l}\,(x,y;X,Z) = 2\mathcal{A}^x_{k-1,l+1} - \mathcal{A}^x_{k-2,l+2} - Z^2\mathcal{A}^x_{k-2,l} + \tfrac{1}{k-1}P_{k-1,l} - X\mathcal{F}^x_{k-2,l}\,(x,y;\Upsilon) \ \text{ for } k \ge 2, \tag{5.12}
$$

where $\Upsilon = X^2 + Z^2$ (cf. (2.1)).

Proof. $\frac{d}{dx}B_{00} = \frac{d}{dx}\frac{1}{Z}\left(\arctan\frac{x-y}{Z} - \arctan\left(\frac{x-y}{Z}\frac{X}{\sqrt{(x-y)^2+\Upsilon}}\right)\right) = \frac{1}{\left(\sqrt{(x-y)^2+\Upsilon}+X\right)\sqrt{(x-y)^2+\Upsilon}} = A_{00}$ yields (5.10), while $A_{10} - A_{01} = \frac{x-y}{\sqrt{(x-y)^2+\Upsilon}\left(X+\sqrt{(x-y)^2+\Upsilon}\right)} = \frac{d}{dx}\ln(X + \sqrt{(x-y)^2 + \Upsilon})$ proves (5.11).

For (5.12) use $A_{k,l} - 2A_{k-1,l+1} + A_{k-2,l+2} + Z^2A_{k-2,l} = \left((x-y)^2 + Z^2\right)A_{k-2,l} = x^{k-2}y^l\frac{\sqrt{(x-y)^2+\Upsilon}-X}{\sqrt{(x-y)^2+\Upsilon}}$ $= x^{k-2}y^l - X\frac{x^{k-2}y^l}{\sqrt{(x-y)^2+\Upsilon}} = x^{k-2}y^l - XF_{k-2,l}$. ■

$$
\mathcal{A}^y_{k,0}\,(x,y;X,Z) = -B_{k,0}\,(x,y;X,Z)\,, \tag{5.13}
$$

$$
\mathcal{A}^y_{k,1}\,(x,y;X,Z) = \mathcal{A}^y_{k+1,0}\,(x,y;X,Z) + M_{k,0}\,(x,y;X,Z)\,, \tag{5.14}
$$

$$
\mathcal{A}^y_{k,l}\,(x,y;X,Z) = 2\mathcal{A}^y_{k+1,l-1} - \mathcal{A}^y_{k+2,l-2} - Z^2\mathcal{A}^y_{k,l-2} + \tfrac{1}{l-1}P_{k,l-1} - X\mathcal{F}^y_{k,l-2}\,(x,y;\Upsilon) \ \text{ for } l \ge 2. \tag{5.15}
$$

Proof. One can transfer the recursions of $\mathcal{A}^x_{k,l}$ as follows to $\mathcal{A}^y_{k,l}$. Note that $A_{k,l}(x,y;X,Z) = A_{l,k}(y,x;X,Z)$ and $M_{k,l}(x,y;X,Z) = M_{l,k}(y,x;X,Z)$. This implies $\mathcal{A}^y_{k,l}(x,y;X,Z) = \mathcal{A}^x_{l,k}(y,x;X,Z)$, where ^{x} (^{y}) denotes the integration with respect to the first (second) argument. ■

Remark 5.1 *To avoid cancellation of terms, we recommend to introduce the related functions*

$$
\begin{aligned}
A'_{kl}\,(x,y;X,Z) &:= (x-y)\,A_{kl}\,(x,y;X,Z) = A_{k+1,l} - A_{k,l+1}, \\
A''_{kl}\,(x,y;X,Z) &:= Z^2 A_{kl}\,(x,y;X,Z)\,.
\end{aligned}
$$

Then, formulae (5.10-5.12) become

$$\mathcal{A}'^{x}_{0,l}(x,y;X,Z) = M_{0,l}(x,y;X,Z),$$
$$\mathcal{A}'^{x}_{k,l}(x,y;X,Z) = \mathcal{A}'^{x}_{k-1,l+1} - \mathcal{A}''^{x}_{k-1,l} + \tfrac{1}{k}P_{k,l} - X\mathcal{F}^{x}_{k-1,l}(x,y;\Upsilon) \text{ for } k \geq 1,$$
$$\mathcal{A}''^{x}_{0,l}(x,y;X,Z) = B''_{0,l}(x,y;X,Z),$$
$$\mathcal{A}''^{x}_{1,l}(x,y;X,Z) = \mathcal{A}''^{x}_{0,l+1}(x,y;X,Z) + Z^2 M_{0,l}(x,y;X,Z),$$
$$\mathcal{A}''^{x}_{k,l}(x,y;X,Z) = 2\mathcal{A}''^{x}_{k-1,l+1} - \mathcal{A}''^{x}_{k-2,l+2} - Z^2\mathcal{A}''^{x}_{k-2,l} + \tfrac{1}{k-1}Z^2 P_{k-1,l} - XZ^2\mathcal{F}^{x}_{k-2,l}(x,y;\Upsilon) \text{ for } k \geq 2,$$

where $B''_{k,l}(x,y;X,Z) := Z^2 B_{k,l}(x,y;X,Z)$. The y-antiderivatives are rewritten similarly. As a consequence, all resulting terms $B_{k,l}$ are replaced by $B''_{k,l}$. Then, formula (2.14) can be replaced by the less dangerous one

$$B''_{k,l}(x,y;X,Y) = Y\left(Q_{k,l}(x,y;Y) - R^{-}_{k,l}(x,y;X,Y)\right).$$

5.5 M

The recursion formulae $\mathcal{M}^{x}_{k,l} \to M_{k+1,l}, \mathcal{A}^{x}_{k',l'}$ and $\mathcal{M}^{y}_{k,l} \to M_{k,l+1}, \mathcal{A}^{y}_{k',l'}$ are formally equal to (5.8), (5.9):

$$\mathcal{M}^{x}_{k,l}(x,y;X,Z) = \frac{M_{k+1,l}(x,y;X,Z) - \mathcal{A}^{x}_{k+2,l}(x,y;X,Z) + \mathcal{A}^{x}_{k+1,l+1}(x,y;X,Z)}{k+1}, \tag{5.16}$$
$$\mathcal{M}^{y}_{k,l}(x,y;X,Z) = \frac{M_{k,l+1}(x,y;X,Z) - \mathcal{A}^{y}_{k,l+2}(x,y;X,Z) + \mathcal{A}^{y}_{k+1,l+1}(x,y;X,Z)}{l+1}. \tag{5.17}$$

Proof. Let $w := \sqrt{(x-y)^2 + \Upsilon}$. The identity $\frac{d}{dx}\left(x^{k+1}\ln(X+w)\right) = (k+1)x^k\ln(X+w) + \frac{x^{k+2}-x^{k+1}y}{w(X+w)}$ shows $\frac{d}{dx}M_{k+1,l} = (k+1)M_{k,l} + A_{k+2,l} - A_{k+1,l+1}$ proving (5.16). ■

In formulae (5.16) and (5.17), the A terms become $-\mathcal{A}'^{x}_{k+1,l}(x,y;X,Z)$ and $\mathcal{A}'^{y}_{k,l+1}(x,y;X,Z)$, respectively, when we apply the choice from Remark 5.1.

5.6 B

Use $\frac{d}{dy}B_{k,l+1} = (l+1)B_{k,l} + x^k y^{l+1}\frac{d}{dy}B_{00} = (l+1)B_{k,l} - A_{k,l+1}$ because of $\frac{d}{dy}B_{00} = -A_{00}$ to obtain

$$\mathcal{B}^{y}_{k,l}(x,y;X,Z) = \frac{B_{k,l+1}(x,y;X,Z) + \mathcal{A}^{y}_{k,l+1}(x,y;X,Z)}{l+1}, \tag{5.18}$$

which is the same recursion as (5.7).

The recursion remains valid when we replace the symbols $A_{k,l}$, $B_{k,l}$ by $A''_{k,l}$, $B''_{k,l}$ (see Remark 5.1).

5.7 D

The auxiliary function $D_{k,l}$ will be needed in the next subsection. The x-integration of $D_{k,l}$ (cf. Lemma 3.14) yields

$$\mathcal{D}^{x}_{0,l}(x,y;Y) = Q_{0,l}(x,y;Y) = y^l \arctan\frac{x-y}{Y}, \tag{5.19}$$
$$\mathcal{D}^{x}_{1,l}(x,y;Y) = YM_{0,l}(x,y;0,Y) + \mathcal{D}^{x}_{0,l+1}(x,y;Y) = \frac{Y}{2}y^l\ln\left((x-y)^2+Y^2\right) + \mathcal{D}^{x}_{0,l+1}, \tag{5.20}$$
$$\mathcal{D}^{x}_{k,l}(x,y;Y) = \frac{1}{k-1}YP_{k-1,l} + 2\mathcal{D}^{x}_{k-1,l+1} - \mathcal{D}^{x}_{k-2,l+2} - Y^2\mathcal{D}^{x}_{k-2,l} \qquad \text{for } k \geq 2. \tag{5.21}$$

Proof. Use $\frac{d}{dx}\frac{Y}{2}y^l\ln\left((x-y)^2+Y^2\right) = Yy^l\frac{x-y}{(x-y)^2+Y^2} = D_{1,l} - D_{0,l+1}$ for $k=1$, while the case $k \geq 2$ follows from $D_{k,l} - 2D_{k-1,l+1} + D_{k-2,l+2} + Y^2 D_{k-2,l} = Yx^{k-2}y^l$. ■

Similarly,

$$\mathcal{D}^{y}_{k,0}(x,y;Y) = -Q_{k,0}(x,y;Y) = -x^k\arctan\frac{x-y}{Y},$$
$$\mathcal{D}^{y}_{k,1}(x,y;Y) = -YM_{k,0}(x,y;0,Y) + \mathcal{D}^{y}_{k+1,0}(x,y;Y) = \frac{Y}{2}x^k\ln\left((x-y)^2+Y^2\right) + \mathcal{D}^{y}_{k+1,0},$$
$$\mathcal{D}^{y}_{k,l}(x,y;Y) = \frac{1}{l-1}YP_{k,l-1} + 2\mathcal{D}^{y}_{k+1,l-1} - \mathcal{D}^{y}_{k+2,l-2} - Y^2\mathcal{D}^{y}_{k,l-2} \qquad \text{for } l \geq 2.$$

5.8 Q

The recursion for $\mathcal{Q}^y_{k,l}$ is identical to those of (5.7) and (5.18):

$$\mathcal{Q}^x_{k,l}(x,y;Y) = \frac{Q_{k+1,l}(x,y;Y) - \mathcal{D}^x_{k+1,l}(x,y;Y)}{k+1},$$
$$\mathcal{Q}^y_{k,l}(x,y;Y) = \frac{Q_{k,l+1}(x,y;Y) + \mathcal{D}^y_{k,l+1}(x,y;Y)}{l+1}. \quad (5.22)$$

Proof. Use $\frac{d}{dx}Q_{k+1,l} = (k+1)\,Q_{k,l} + D_{k+1,l}$ and $\frac{d}{dy}Q_{k,l+1} = (l+1)\,Q_{k,l} - D_{k,l+1}$. ■

5.9 R,E

Since $R^-_{k,l}$ and $E^-_{k,l}$ are obtained from $R^+_{k,l}$ and $E^+_{k,l}$ by swopping the roles of the parameters X, Y, it suffices to discuss $R^+_{k,l}$ and $E^+_{k,l}$. Their x-antiderivatives are obtained by the combined recursions

$$\mathcal{R}^{+x}_{0,l}(x,y;X,Y) = R^+_{1,l} - R^+_{0,l+1} - E^+_{0,l}, \quad (5.23)$$
$$\mathcal{E}^{+x}_{0,l}(x,y;X,Y) = E^+_{1,l} - E^+_{0,l+1} + X^2R^+_{0,l} - XY\mathcal{F}^x_{0,l}(x,y;\Theta), \qquad \Theta = X^2+Y^2, \quad (5.24)$$
$$\mathcal{R}^{+x}_{k,l}(x,y;X,Y) = \frac{R^+_{k+1,l} - R^+_{k,l+1} - E^+_{k,l} + k\mathcal{R}^{+x}_{k-1,l+1} + k\mathcal{E}^{+x}_{k-1,l}}{k+1} \quad \text{for } k \geq 1, \quad (5.25)$$
$$\mathcal{E}^{+x}_{k,l}(x,y;X,Y) = \frac{E^+_{k+1,l} - E^+_{k,l+1} + X^2R^+_{k,l} + k\mathcal{E}^{+x}_{k-1,l+1} - X^2k\mathcal{R}^{+x}_{k-1,l} - XY\mathcal{F}^x_{k,l}}{k+1} \quad \text{for } k \geq 1. \quad (5.26)$$

Proof. The following proof uses

$$\frac{d}{dx}E^+_{00} = XY\frac{x-y}{\sqrt{\Theta+(x-y)^2}\left(X^2+(x-y)^2\right)}, \quad \frac{d}{dx}R^+_{00} = XY\frac{1}{\sqrt{\Theta+(x-y)^2}\left(X^2+(x-y)^2\right)}. \quad (5.27)$$

(5.23) and (5.24) are the cases $k=0$ of the following formulae.

Use $\frac{d}{dx}\left(R^+_{k+1,l} - R^+_{k,l+1} - E^+_{k,l}\right) = (k+1)\,R^+_{k,l} - kR^+_{k-1,l+1} - kE^+_{k-1,l} + x^ky^l\left[(x-y)\frac{d}{dx}R^+_{00} - \frac{d}{dx}E^+_{00}\right]$ and note that $[\ldots] = 0$ because of (5.27). This proves (5.25).

The identity $x^ky^l\left[(x-y)\frac{d}{dx}E^+_{00} + X^2\frac{d}{dx}R^+_{00}\right] = XYF_{k,l}$ implies $\frac{d}{dx}\left((x-y)\,E^+_{k,l} + X^2R^+_{k,l}\right) = (k+1)\,E^+_{k,l} - kE^+_{k-1,l+1} + X^2kR^+_{k-1,l} + XYF_{k,l}$ proving (5.26). ■

Similarly,

$$\mathcal{R}^{+y}_{k,0}(x,y;X,Y) = -R^+_{k+1,0} + R^+_{k,1} + E^+_{k,0},$$
$$\mathcal{E}^{+y}_{k,0}(x,y;X,Y) = -E^+_{k+1,0} + E^+_{k,1} - X^2R^+_{k,0} - XY\mathcal{F}^y_{k,0}(x,y;\Theta), \qquad \Theta = X^2+Y^2,$$
$$\mathcal{R}^{+y}_{k,l}(x,y;X,Y) = \frac{-R^+_{k+1,l} + R^+_{k,l+1} + E^+_{k,l} + l\mathcal{R}^{+y}_{k+1,l-1} - l\mathcal{E}^{+y}_{k,l-1}}{l+1} \quad \text{for } l \geq 1,$$
$$\mathcal{E}^{+y}_{k,l}(x,y;X,Y) = \frac{-E^+_{k+1,l} + E^+_{k,l+1} - X^2R^+_{k,l} + l\mathcal{E}^{+y}_{k+1,l-1} + X^2l\mathcal{R}^{+y}_{k,l-1} - XY\mathcal{F}^y_{k,l}}{l+1} \quad \text{for } l \geq 1.$$

5.10 C

The relation $C'_{k,l} = Q_{k+1,l} - Q_{k,l+1}$ (cf. (2.8)) yields

$$\mathcal{C}'^x_{k,l}(x,y;Y) = \mathcal{Q}^x_{k+1,l}(x,y;Y) - \mathcal{Q}^x_{k,l+1}(x,y;Y). \quad (5.28)$$

Similarly, $C^\pm_{k,l} = (x-y)\,R^\pm_{k,l} = R^\pm_{k+1,l} - R^\pm_{k,l+1}$ leads to

$$\mathcal{C}^{\pm x}_{k,l}(x,y;X,Y) = \mathcal{R}^{\pm x}_{k+1,l}(x,y;X,Y) - \mathcal{R}^{\pm x}_{k,l+1}(x,y;X,Y).$$

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6 Appendix: The Program `coulomb`

The program `coulomb` allows to perform the operations described before. The source code exists as Pascal program `coulomb.pas` as well as C program `coulomb.c`. Since the latter is automatically translated from the former one, the Pascal source text is better readable. Both programs are obtainable from `http://???`

6.1 First Test Example

We show how the first example from §3.14 can be obtained. After starting the program, the main menu arises, which contains a subset[6] of the following options:

	MAIN MENU
1	`define actual function expression`
2	`integration`
3	`evaluation`
4	`interpretation of the function w.r.t.` $x_2, y_2/x_3, y_3$
5	`output and storage of actual function expression`
6	`internal status`
7,l	`list the actual function expression`
blank	`end of program`

The options 1,2,3,5,6 lead to sub-menus which are described in detail below. We use the notation *Option(1f)* for the result of selecting "1" in the main menu and "f" in the arising sub-menu. Similarly, a sequence of options is written as *Option*($a_1b_1, a_2b_2, \dots$), where a_i, b_i are characters.

The first test example consists of the options *Option(1f,22,31,4,22,31,4,22,33,6n)*. The resulting number 0.980885... is the result given in §3.14.

Step	*main menu*	*sub-menu*	*comment*
1)	1	f	define *expression* $:= F = 1/\sqrt{(x-y)^2 + X^2 + Y^2}$
2)	2	2	perform x- and y-integration $(x = x_1, y = y_1)$
3)	3	1	evaluate at $\dots\vert_{x=0}^{x=1}\vert_{y=0}^{y=1}$ $(x = x_1, y = y_1)$
4)	4		interprete as function w.r.t. x_2, y_2
5)	2	2	perform x- and y-integration $(x = x_2, y = y_2)$
6)	3	1	evaluate at $\dots\vert_{x=0}^{x=1}\vert_{y=0}^{y=1}$ $(x = x_2, y = y_2)$
7)	4		interprete as function w.r.t. x_3, y_3
8)	2	2	perform x- and y-integration $(x = x_3, y = y_3)$
9)	3	3	evaluate at $\dots\vert_{x=1}^{x=2}\vert_{y=0}^{y=1}$ $(x = x_3, y = y_3)$
10)	5	n	compute the numerical value `0.9808851836009822`

(6.1)

6.2 First Test Continued: Further Output

After each step in (6.1) the actual expression can be shown by means[7] of *Option(7)*. Before Step 1) it produces the answer `ZERO`. After Step 1) the result is $+\{[+(1)]\} * F(x-y; Y, Z)$, while after Step 2) *Option(7)* yields

$$
\begin{aligned}
&+\{[+(2) * Z\hat{}2] * x + [+(-2) * Z\hat{}2] * y\} * B(x-y; +(0), Z) \qquad (6.2)\\
&+\{[+(-2) * Z\hat{}2] * x + [+(2) * Z\hat{}2] * y\} * B(x-y; +(1), Z)\\
&+\{[+(2/3) * Z\hat{}2] + [+(-1/3)] * x\hat{}2 + [+(2/3)] * x * y + [+(-1/3)] * y\hat{}2\} * G(x-y; +(0), Z)\\
&+\{[+(1/3) + (-2/3) * Z\hat{}2] + [+(1/3)] * x\hat{}2 + [+(-2/3)] * x * y + [+(1/3)] * y\hat{}2\} * G(x-y; +(1), Z)\\
&+\{[+(-1) * Z\hat{}2] * x + [+(1) * Z\hat{}2] * y\} * L(x-y; +(0), Z)\\
&+\{[+(-1) + (1) * Z\hat{}2] * x + [+(1) + (-1) * Z\hat{}2] * y\} * L(x-y; +(1), Z)\\
&+\{[+(-1) * Z\hat{}2] + [+(1)] * x\hat{}2 + [+(-2)] * x * y + [+(1)] * y\hat{}2\} * M(x-y; +(0), Z)\\
&+\{[+(1) * Z\hat{}2] + [+(-1)] * x\hat{}2 + [+(2)] * x * y + [+(-1)] * y\hat{}2\} * M(x-y; +(1), Z)
\end{aligned}
$$

[6] Only those options are shown which are reasonable in the present situation. Although the other options are selectable, their result may lead to wrong results.

[7] *Option(7)* and *Option(l)* are identical. The character `l` is used for the same purpose in many of the sub-menus.

which[8] is identical to (3.7). The notation $B(x-y;+(0),Z)$ is used instead of $B_{00}(x,y;0,Z)$, since x,y appear only as the difference. It is multiplied by the preceding polynomial $\{\dots\}$. Each term of this polynomial is written as $[\dots]*x\hat{\ }k*y\hat{\ }l$. The notation of the monomial $x\hat{\ }k$ is omitted when $k=0$ and abbreviated by x when $k=1$. The expression (6.2) is also written into the protocol file *coulomb.log.*

In the end, when all parameters are evaluated, the result can be transferred into TEX format. After Step 9), *Option(5t)* produces the file *coulomb.tex* which then contains

$$\begin{aligned}
&-\frac{4}{15}-\frac{1}{3}*\sqrt{2}+\frac{4}{5}*\sqrt{3}+\frac{16}{15}*\sqrt{4}-\frac{2}{3}*\sqrt{5}-\frac{3}{5}*\sqrt{6} \\
&+\frac{8}{3}*\ln\left(\sqrt{2}\right)-\frac{16}{3}*\ln\left(\sqrt{4}\right)-\frac{7}{3}*\ln\left(\sqrt{5}\right)-\frac{5}{3}*\ln\left(1+\sqrt{2}\right) \\
&-4*\ln\left(1+\sqrt{3}\right)+\frac{16}{3}*\ln\left(1+\sqrt{5}\right)+\frac{7}{3}*\ln\left(1+\sqrt{6}\right)+\frac{2}{3}*\ln\left(2+\sqrt{5}\right)+\frac{4}{3}*\ln\left(2+\sqrt{6}\right) \\
&-2*\pi+8*\arctan\left(2*\frac{1}{\sqrt{6}}\right)
\end{aligned} \tag{6.3}$$

as TEX expression. One may check that (6.3) is equal to the value I_{face} given in §3.14, although the terms are not identical.

6.3 Sub-Menu for Output

After the previous examples, we discuss in detail the following sub-menu (called by *Option(5)*):

	MENU for output and storage of the actual function expression
	screen ...
`l`	`list the actual value of the expression`
`n`	`compute the numerical value of the expression`
	internal ...
`s`	`write into internal storage`
	external ...
`t`	`write into TEX file` <*name*>
`x`	`write into external storage` <*name*>
`blank`	`return to main menu`

(6.4)

- Option `l`: It produces a display at the screen and a printout into the protocol file whose standard name is *coulomb.log.* This name may be changed by *Option(6p).*
- Option `n`: Only possible if all parameters are evaluated. Then it computes the numerical value of the actual expression, which is a sum like in (6.3). To check the possible influence of floating-point errors, also the sum of the moduli of all terms is given. In the case of (6.3), the latter sum is 43.07... Assuming a maschine precision $eps = 2.2_{10}$-16, the rounding error effect should be bounded by 1_{10}-14 so that the last two digits in `0.9808851836009822` are in doubt.
- Option `s`: The actual expression is memorised internally. *Option(1s)* returns the expression.
- Option `t`: Only possible if all parameters are evaluated. Then it translates the expression into TEX format and writes it into a file whose standard name is *coulomb.tex.* The actual name <*name*>is written in the menu line. This name can be changed any time by *Option(6t).*
- Option `x`: The actual expression is stored onto a file whose standard name is *coulomb.ext.* The actual name <*name*>is written in the menu line. This name can be changed any time by *Option(6x).* For reading the stored expression use *Option(1x).*

6.4 Notation of Variables

The notation of the variable and parameter names must be defined more explicitly.

[8]The original output uses much more but shorter lines. The reason for having one separate line for each term is that the number of terms in the polynomials is not limited.

The function $F_{k,l}$ is defined in (2.2) by means of $\Xi = Y^2 + Z^2$. Now we use Y, Z explicitly and add the parameter ξ :

$$F_{k,l}(x, y; X, Y) = \frac{x^k y^l}{\sqrt{(x-y)^2 + X^2 + Y^2}}. \tag{2.2*}$$

Here, X, Y are the generic names for the parameter variables. Due to the interpretation by $\Xi = Y^2 + Z^2$, we may associate the symbol "Y" to X and the symbol "Z" to Y.

Remark 6.1 *The notation of the variables for the following functions will be always $x, y; X, Y$, unless the function does not depend of some of these variables (as, e.g., the polynomial $P_{k,l}(x, y)$). Depending on what integration step we are considering, the meaning of these variables might be different. For instance, x, y are understood as x_i, y_i in integration phase i $(1 \le i \le 3)$.*

The meaning of X, Y is given by its symbols $\sigma(X), \sigma(Y)$ (e.g., $\sigma(X) =$ "Y", $\sigma(Y) =$ "Z" according to (2.1)).

As long as $\sigma(X) =$ "Y", X carries no value. In the case of an evaluation, we redefine $\sigma(X) =$ "" (empty name) and X cannot be treated symbolically any longer.[9]

6.5 Reformulated Recursion Formulae

Similar to $F_{k,l}$, we write

$$G_{k,l}(x, y; X, Y) = x^k y^l \sqrt{(x-y)^2 + X^2 + Y^2}\,, \tag{2.3*}$$

$$L_{k,l}(x, y; X, Y) = x^k y^l \ln\left(x - y + \sqrt{(x-y)^2 + X^2 + Y^2}\right). \tag{2.4*}$$

The recursion formulae for the integrals of F are to be adjusted whenever Ξ appears, as in (5.3), (5.6):

$$\mathcal{F}^x_{k,l} = \frac{G_{k-1,l} + (2k-1)\,\mathcal{F}^x_{k-1,l+1} - (k-1)\,\mathcal{F}^x_{k-2,l+2} - (k-1)\left(X^2+Y^2\right)\mathcal{F}^x_{k-2,l}}{k} \quad \text{for } k \ge 2, \tag{5.3*}$$

$$\mathcal{F}^y_{k,l} = \frac{G_{k,l-1} + (2l-1)\mathcal{F}^y_{k+1,l-1} - (l-1)\mathcal{F}^y_{k+2,l-2} - (l-1)\left(X^2+Y^2\right)\mathcal{F}^y_{k,l-2}}{l} \quad \text{for } l \ge 2, \tag{5.6*}$$

where all functions have the arguments $(x, y; X, Y, \xi)$. The formulae (5.1/2/4/5) and (5.7-9) for G, L stay valid when we replace the argument list $(x, y; \Xi)$ by $(x, y; X, Y)$.

Remark 6.2 *The recursion (5.3*) is managed differently when X represents a symbolic variable or a given real number. In the first case, the coefficients of the functions are polynomials also in X, while in the second case, the real number is used instead. Obviously, the amount of work and the length of the resulting expression is reduced a lot, when we evaluate X as soon as possible.*

We follow the device in Remark 5.1 and use A'_{kl}, A''_{kl} instead of A_{kl} and $B''_{k,l}$ instead of B_{kl}.

The translation of the function names introduced so far and the names used in the program and output is given in the following list.

mathematical name	program	mathematical name	program
$A'_{00}\,(x, y; X, Y)$	DA(x-y;X,Y)	$A'_{00}\,(x, y; X, Y)$	AZ(x-y;X,Y)
$B''_{00}\,(x, y; X, Y)$	BZ(x-y;X,Y)	$C'_{00}\,(x, y; X, Y)$	C0(x-y;X,Y)
$C^+_{00}\,(x, y; X, Y)$	Cp(x-y;X,Y)	$C^-_{00}\,(x, y; X, Y)$	Cm(x-y;X,Y)
$D_{00}\,(x, y; Y)$	D(x-y;Y)		
$E^+_{00}\,(x, y; X, Y)$	Ep(x-y;X,Y)	$E^-_{00}\,(x, y; X, Y)$	Em(x-y;X,Y)
$F_{00}\,(x, y; X, Y)$	F(x-y;X,Y)	$G_{00}\,(x, y; X, Y)$	G(x-y;X,Y)
$L_{00}\,(x, y; X, Y)$	L(x-y;X,Y)	$M_{00}\,(x, y; X, Y)$	M(x-y;X,Y)
$P_{00}\,(x, y)$	1	$P^s_{00}\,(x, y)$	π/2*sign(x-y)
$Q_{00}\,(x, y; Y)$	Q(x-y;Y)		
$R^+_{00}\,(x, y; X, Y)$	Rp(x-y;X,Y)	$R^-_{00}\,(x, y; X, Y)$	Rm(x-y;X,Y)

(6.5)

Furthermore, if x, y are evaluated, we chance "π/2*sign(x-y)" into a factor times "π".

[9] In the program, the empty file is replaced by "$" because of better visibility.

6.6 Internal Representation

In the following, the sub-menu called by *Option(6)* is of interest:

	MENU for internal variables
`l`	`list status of internal variables`
	representation for output ...
`f`	`use floating point numbers`
`r`	`use rational numbers`
`T`	`change value of Tolerance`
`q`	`change value of TolRational`
`a`	`change value of MaxDenominator`
	files ...
`t`	`change name of external TEX file`
`x`	`change name of external storage file`
`p`	`change name of protocol file`
	for further choices see output produced by "`l`"
`blank`	`return to main menu`

(6.6)

Option(6t), Option(6x), and *Option(6p)* are already mentioned in §6.3. The other options are explained below.

6.6.1 Format of real numbers

All (non-zero) coefficients are internally represented by standard floating point numbers. In the procedure *SparsifyPolynomial*, where zero terms are omitted from the list, all real numbers with

$$|x| \leq Tolerance \tag{6.7}$$

are treated as zeros. The standard value of this constant is $Tolerance = 100 * MachineEps$, where the machine precision $MachineEps$ is a constant (the used value $MachineEps$=2.2E-16 should be adapted to the actual computer). Change the value of $Tolerance$ into zero, if the rounding to zero should be avoided. A redefinition of $Tolerance$ is possible by *Option(6T)*.

Since the recursion formulae use only simple rational numbers as coefficients, the exact result of the computations are also rational, provided that also the possible values at which the variables are evaluated are also simple rationals. By this reason we provide an output, where all reals are interpreted as rationals. *Option(6r)* allows to choose this representation (standard option). Otherwise, after *Option(6f)*, the floating point number representation is used for the output.

In the case of rational output, the rational number n/m has the property that $|x - \frac{n}{m}| \leq TolRational$ and $0 < m \leq MaxDenominator$. If such an $\frac{n}{m}$ is not found or if $|x| < TreatAsRationalNumber$, x is represented as floating point real. To redefined $TolRational$ or $MaxDenominator$ use *Option(6q)* or *Option(6a)*, respectively[10].

Another constant, which should be adapted to the actual machine, is the maximal long integer number $maxLongInteger$. This value is used to check whether $abs(x * m) > maxLongInteger$. In the positive case, the corresponding rational number $\frac{n}{m}$ is not representable since n exceeds $maxLongInteger$.

Option(6l) shows all internal parameters.

Again we remark that the choice of the various parameters except $Tolerance$ concerns only the output, while the (quality of the) computation is not influenced. The rounding due to (6.7) makes sense, because of the rational nature of the exact results. Very small non-vanishing numbers are not expected as true results but should result from the cancellation of equal rationals. Here, we recommend to scale the problems such that the coefficients are expected in the size $O(1)$.

6.6.2 Function Representation

The computation deals with expressions of the form

$$\Phi(x, y; X, Y) = \sum_{i,k,l} c_{i,k,l} \Phi^i_{k,l}(x, y; X, Y). \tag{6.8}$$

[10]The value $TreatAsRationalNumber := 1/(MaxDenominator + 1)$ depends only on the choice of $MaxDenominator$.

In the program, this expression is represented by a list (the index i in corresponds to the ith list element). Here, Φ^i for different i represents different function names $F, G, \ldots$ and possibly different evaluations. The lower index in $\Phi^i_{k,l}$ has the meaning $x^k y^l$, i.e., $\Phi^i_{k,l} = x^k y^l \Phi^i_{0,0}$ as already used for $F_{k,l}, \ldots$. Therefore, we rewrite the above expression as

$$\sum_{i,k,l} c_{i,k,l} x^k y^l \Phi^i(x,y;X,Y) = \sum_i \left(\sum_{k,l} c_{i,k,l} x^k y^l \right) \Phi^i(x,y;X,Y), \tag{6.9}$$

where Φ^i is a short notation for $\Phi^i_{0,0}$. The resulting coefficient $\sum_{k,l} c_{i,k,l} x^k y^l$ is a polynomial described in the next subsection.

If the parameters $x, y; X, Y$ are symbolic, the different indices i correspond to different function names from Table (6.6). As soon as parameters are evaluated, we must distinguish, e.g., between $F(x,y;X,0)$ and $F(x,y;X,1)$. Hence, different evaluations appearing in (6.8) get different indices i, i.e., they are represented by different elements in the list (compare the listing (6.2)).

The output of an expression (6.8) is a sum of terms of the form $Polynomial(x,y,X,Y) * FunctionName$. The meaning of the function names is explained in (6.6).

Remark 6.3 *a) Since all functions depend on the difference $x - y$, this difference is used in the output.*

b) The variables x, y, X, Y are named by their symbols or when evaluated by their values (e.g., F(1-x;1,Z)).

c) The internal function name of P_{00} is P. Similarly, the names Ps and Pi is used for $P^s_{00}(x,y)$ and π.

d) The procedure stabilise *tries to convert some of these functions into other ones, so that the output will not contain all function types although they have been produced by the recursion formulae.*

The conversions mentioned in Remark 6.3d concern

	from		into	under the condition	
a)	$L(\cdot;X,Y)$	$\to$	$L(\cdot;Y,X)$	$X > Y$ evaluated	(same for F,G)
b)	$F(\delta;X,\cdot)$	$\to$	$F(X;\delta,\cdot)$	$\delta = x - y > X$ evaluated	(same for G)
c)	$M(\delta;X,Y)$	$\to$	$L(X;\delta,Y)$	δ, X evaluated	
d)	$Cm(\cdot;X,Y)$	$\to$	$Cp(\cdot;Y,X)$		(same for Em)
e)	M(·;X,Y)	$\to$	$-$M(·;-X,Y) + 2*M(·;0,Y)	$X < 0$ evaluated	(cf. (3.3))
f)	L(δ;X,Y)	$\to$	$-$L(-δ;-X,Y) + 2*L(0;X,Y)	$\delta < 0$ evaluated	

(6.10)

The standard choice is that a-f) are allowed, where d) is restricted to the case when X, Y are evaluated. By *Option(6G)*, *Option(6g)*, *Option(6m)*, *Option(6c)* we may stop the conversions. On the other hand, *Option(6X)* allows the conversion d) even if X, Y are not evaluated. This, however, leads to wrong results when at the end of Phase 2, *Option(4)* tries to interpret the expression as a function of $Y = x_3 - y_3$, since Y is expected in the fourth parameter place.

6.6.3 Polynomial Representation

The coefficients in (6.9) are polynomials of the form

$$\sum_{k,l} c_{k,l}(X,Y) x^k y^l, \tag{6.11}$$

where the coefficients $c_{k,l}(X,Y)$ are again standard real polynomials in X, Y :

$$c(X,Y) = \sum_{k,l} \zeta_{k,l} X^k Y^l \qquad (\zeta_{k,l} \in \mathbb{R}). \tag{6.12}$$

In the program, expressions of the form (6.12) are associated with $level = 0$, while polynomials (6.11) correspond to $level = 1$. Mathematically, we are able to express all polynomials in four variables x, y, X, Y.

Similar to Remark 6.2, the computing time and the length of the expressions is reduced when we evaluate some of the variable by a real value. For instance, the evaluation $X := \xi$ and $Y := \eta$ replaces the possibly lengthy polynomial $c(X,Y)$ by the constant polynomial $\zeta_{0,0} = c(\xi,\eta)$.

Since the polynomials are represented by lists of the non-vanishing terms, we have no bounds for the maximal polynomial degree (except storage limitations).

6.7 Function Input

The following sub-menu called by *Option(1)* allows to define or change the actual expression:

	MENU for defining the actual function expression
	standard start ...
f	define expression by F and return to phase:=1
	special ...
a	add a term $polynomial * function$
0	set expression to zero
m	multiply by a polynomial (subject of input)
	from storage ...
s	take from internal storage (expression overwritten by storage content)
+	add from internal storage (expression := expression + storage)
x	read from external storage "<*name*>"
	other actions ...
l	list the actual value of the expression
b	stabilisation and further simplifications
o	omit zero terms, combine suitable terms
p	change phase number
blank	return to main menu

- Option `f`: actual expression := $F_{00}(x-y;X,Y)$ (with symbolic x,y,X,Y). Further $Phase := 1$ is defined (see §6.8.2). After this (standard) option, the program return immediately to the main menu. After all other options, the program does not leave this sub-menu.
- Option `a`: The term $Polynomial(x,y,X,Y) * FunctionName$ defined during this action is added to the actual expression. First, the program asks for the name of the function, which is DA,AZ,... as in Table (6.5). Additionally, P, Pi and Ps represent $P_{00}, \pi * P_{00}$ and P_{00}^s. Next, the program asks for the polynomial (see §6.7.1).
- Option `0`: The actual expression is replaced by zero.
- Option `m`: The program asks for a polynomial $p(x,y;X,Y)$. The product of the actual expression and the input polynomial defines the new expression. This action corresponds to the Steps 2a,3a from §3.16.
- Option `s`: The expression previously stored by *Option(5s)* into the internal storage becomes the actual expression.
- Option `+`: The internally stored expression is added to the actual one.
- Option `x`: The expression previously stored by *Option(5x)* into the external storage becomes the actual expression. The file name of external storage is given in the menu line. Note that this name can be changed by *Option(6x)*.
- Option `l`: As *Option(5l)*. Although this is an output action, it is added here to check the input expression.
- Option `b`: The procedure *stabilise* produces the conversions (6.10). Furthermore, coefficients satisfying (6.7) are omitted. Usually, this procedure is implicitly called.
- Option `o`: This is a weaker form of the previous option, i.e., no conversions are performed, only zero terms are omitted and terms with equals function names are added into one term.
- Option `p`: The actual expression is unchanged, only the phase number is redefined (see §6.8.2).

6.7.1 Polynomial Input

An explicit input of polynomials of the form (6.11) happens in the second part of *Option(1a).* The input of the polynomial $p(x, y; X, Y) = 1 + \left(3 + 4X^2\right) y^2$ requires the following dialogue, in which the bold-face part indicates the input. The text on the right-hand side are additional comments.

### input of polynomial ...	level-1-polynomial started
choose the degrees k, l <terminate with $k < 0$ >	
->k = **0**	
->l = **0**	x^0y^0
choose "0" for real coefficient (constant polynomial) or	
"1" for non-constant polynomial. Choice = 0	
->value of coefficient[0,0] = 1	constant term 1 defined
choose the degrees k, l <terminate with $k < 0$ >	
->k = **0**	
->l = **2**	x^0y^2
choose "0" for real coefficient (constant polynomial) or	
or "1" for non-constant polynomial. Choice = 1	
##### input of coefficient polynomial ...	level-0-polynomial started
choose the degrees k, l <terminate with $k < 0$ >	
->k = **0**	
->l = **0**	X^0Y^0
->value of coefficient[0,0] = 3	constant term 3 defined
choose the degrees k, l <terminate with $k < 0$ >	
->k = **2**	
->l = **0**	X^2Y^0
->value of coefficient[2,0] = 4	2nd term $4X^2$ defined
choose the degrees k, l <terminate with $k < 0$ >	
->k = **-1**	
value must be non-negative	
##### input of coefficient polynomial finished	level-0-polynomial defined
choose the degrees k, l <terminate with $k < 0$ >	
->k = **-1**	
value must be non-negative	
### input of polynomial finished	level-1-polynomial defined

6.8 Integration and Phases

6.8.1 Integration

Integration with respect to x or y is possible as long as the respective variables are symbolic. *Option(2)* leads to the corresponding sub-menu.

	MENU for integration
	integration ...
`2`	`xy-integration including stabilisation`
`x`	`x - integration followed by stabilisation`
`X`	`. . . . . without stabilisation`
`y`	`y - integration followed by stabilisation`
`Y`	`. . . . . without stabilisation`
	other actions ...
`l`	`list actual expression`
`b`	`stabilisation and further simplifications`
`o`	`omit zero terms, combine suitable terms`
`blank`	`return to main menu`

- Option `0`: This is the standard choice, combining the options `x,y,` i.e., the x- and y-integration are performed including stabilisation (call of *stabilise* as discussed in Remark 6.3d).
- Option `x`: The x-integration is performed including stabilisation.
- Option `X`: The x-integration is performed without stabilisation. This is of interest, if one wants to see the direct result of the recursion formulae.
- Option `y`: The x-integration is performed including stabilisation.
- Option `Y`: The y-integration is performed without stabilisation.
- Options `l,b,o`: Identical to *Option(1l), Option(1b), Option(1o).*

As soon as the x- and y-integration are performed, the program returns directly to the main menu.

6.8.2 Phases and Functions Reinterpretation

The Phases 1 to 3 are characterised by the fact that the integration can be performed with respect to the variables $x = x_i$, $y = y_i$ $(1 \leq i \leq 3)$. The meaning of the parameters X, Y changes in each phase:

Phase	meaning of X	meaning of Y	$\sigma(X)$	$\sigma(Y)$
1	$x_2 - y_2$ (symbolic)	$x_3 - y_3$ (symbolic)	"Y"	"Z"
2	$x_1 - y_1$ (evaluated)	$x_3 - y_3$ (symbolic)	"X"	"Z"
3	$x_1 - y_1$ (evaluated)	$x_2 - y_2$ (evaluated)	"X"	"Y"

(6.13)

The output uses the symbols $\sigma(X)$, $\sigma(Y)$ from this table, but note that, e.g., in Phase 3 under regular assumptions these symbol should not appear, since the parameters are already evaluated.

The program is starting with Phase 1. Phase 1 is concluded by the reinterpretation *Option(4)*, which leads[11] to a function in x_2, y_2. *Option(4)* requires that the x, y-variables are evaluated, while the parameter X is still symbolic.

After the reinterpretation the phase number is 2. Due to the assumptions from above, the requirement "$x_1 - y_1$ evaluated" from (6.13) is satisfied. Phase 2 allows to integrate and evaluate with respect to $x = x_2, y = y_2$. As soon as x, y are evaluated (and $Y =$ "Z" is still symbolic), we may call *Option(4)*, which now leads to a function in x_3, y_3 in Phase 3 (the only free variables are $x = x_3, y = y_3$).

We add that the phase numbers can be changed by *Option(1p)*. This allows to jump from Phase 1 (starting situation) immediately into Phase 2. Then, e.g., the function $M_{00}(x, y; X; Y)$ can be defined (*by Option(1a)*) and its x, y-antiderivative can be determined (by *Option(22)*). In the latter, case the variable X is symbolic which is different from the standard situation in (6.13).

Remark 6.4 *a) The exact conditions for* Option(4) *in Phase 1 (transition from Phase 1 to 2) are: x, y-variables evaluated and $X =$ "Y" symbolic. The status of the variable $Y =$ "Z" is not of interest. For instance, $Y = \xi$ may be already evaluated to compute the 2D-integral*

$$\iint_{R'} \iint_{R''} \frac{x_1^{\nu_1} x_2^{\nu_2} y_1^{\mu_1} y_2^{\mu_2}}{\sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \xi^2}} dx_1 dy_1 dx_2 dy_2.$$

b) Option(4) *in Phase 2 (transition from Phase 2 to 3) requires: x, y- and X-variables evaluated and $Y =$ "Z" symbolic.*

[11] More precisely, the old expression $\Phi(x, y; X, Y) \equiv \Phi(x_1, y_1; \text{“}Y\text{”}, \text{“}Z\text{”})$ is replaced by $\tilde{\Phi}(x, y; X, Y) \equiv \tilde{\Phi}(x_2, y_2; x_1 - y_1, \text{“}Z\text{”}) := \Phi(x_1, y_1; x_2 - y_2, \text{“}Z\text{”})$. Here, we have used that after evaluation of x_1, y_1 in $\Phi(x_1, y_1; \text{“}Y\text{”}, \text{“}Z\text{”})$, this is expressed by a linear combination (6.8) with $\sum_{k,l} c_{i,k,l} x_1^k y_1^l = c_{i,0,0} = c_{i,0,0}(X, Y)$ and the functions $\Phi^i(x_1, y_1; X, Y)$ in (6.8) depend only of the difference $x_1 - y_1$, which becomes the value of X in $\tilde{\Phi}(x, y; X, Y)$. The old X parameter appearing in the functions $\Phi^i(x_1, y_1; X, Y)$ as well as in the coefficients $c_{i,0,0}(X, Y)$ is substituted by $x_1 - y_1$. Since $c_{i,0,0}(X, Y)$ is a polynomial in X, Y, the substitution yields a new polynomial in $x = x_2, y = y_2$ and Y.

6.9 Evaluation

Option(3) yields the sub-menu, which offers various possibilities for the evaluation of the parameters.

	MENU for evaluation
	evaluation of x ...
x	replace x by a real value (value is subject of input)
i	. . . . . $p(x,y)$ by $p(x2,y)-p(x1,y)$ for real values $x1,x2$
	... same without stabilisation ...
a	`replace` x `by a real value`
A	. . $p(x,y)$ `by` $p(x2,y)-p(x1,y)$ `for real values` $x1,x2$
	evaluation of y ...
y	`replace` y `by a real value (value is subject of input)`
j	. . $p(x,y)$ `by` $p(x,y2)-p(x,y1)$ `for real values` $y1,y2$
	... same without stabilisation ...
b	`replace` y `by a real value`
B	. . $p(x,y)$ `by` $p(x,y2)-p(x,y1)$ `for real values` $y1,y2$
	evaluation of x and y ...
c	. . `combine actions ''x'' and ''y''`
1	. . x=0,1 and y=0,1
2	. . x=0,1 and y=1,2
3	. . x=1,2 and y=0,1
4	. . x=1,2 and y=1,2
	evaluation of parameters X or Y ...
X	`replace` $\sigma(X)$ `by a real value`
Y	`replace` $\sigma(Y)$ `by a real value`
	other actions ...
l	`list actual expression`
blank	`return to main menu`

- Option `x`: Only possible if x is a symbolic variable. The expression $\Phi(x,\cdot;\cdot,\cdot)$ is replaced by $\Phi(a,\cdot;\cdot,\cdot)$, where the real number a is the input during this action. A following call of *stabilise* leads to a simplification and stabilisation (cf. 6.3d).
- Option `i`: Only possible if x is a symbolic variable. The expression $\Phi(x,\cdot;\cdot,\cdot)$ is replaced by $\Phi(x,\cdot;\cdot,\cdot)|_{x=a}^{x=b}$ with following stabilisation.
- Option `y,j`: Analogous actions concerning the y-variable.
- Option `a,A,b,B`: Same as `x,i,y,j` but without stabilisation.
- Option `c`: The combination of `x` and `y`, i.e., $\Phi(x,y;\cdot,\cdot)$ is replaced by $\Phi(x,y;\cdot,\cdot)|_{x=a}^{x=b}|_{y=c}^{y=d}$ with following stabilisation.
- Option `1`: Model case $\Phi(x,y;\cdot,\cdot)|_{x=0}^{x=1}|_{y=0}^{y=1}$, i.e. Option `c` with $a=c=0$, $b=d=1$.
- Option `2`: Model case $\Phi(x,y;\cdot,\cdot)|_{x=0}^{x=1}|_{y=1}^{y=2}$, i.e. Option `c` with $a=0$, $b=c=1$, $d=2$.
- Option `3`: Model case $\Phi(x,y;\cdot,\cdot)|_{x=1}^{x=2}|_{y=0}^{y=1}$, i.e. Option `c` with $c=0$, $a=d=1$, $b=2$.
- Option `4`: Model case $\Phi(x,y;\cdot,\cdot)|_{x=1}^{x=2}|_{y=1}^{y=2}$, i.e. Option `c` with $a=c=1$, $b=d=2$.
- Option `X`: Only possible if X is a symbolic variable. The expression $\Phi(\cdot,\cdot;X,\cdot)$ is replaced by $\Phi(\cdot,\cdot;a,\cdot)$, where the real number a is the input during this action.
- Option `Y`: Analogous action concerning the Y-variable.
- Option `l`: As *Option(5l)*.

Remark 6.5 *The evaluation concerns only those terms in (6.8) where the corresponding variable is not yet evaluated. This is important, since for instance the expression may contain $M(x,y;X,Y)$ as well as $M(x,y;0,Y)$. Then the evaluation of X at ξ must not change $M(x,y;0,Y)$.*

6.10 A further Test Example

In the introduction we mentioned the case $B' = [0,100] \times [0,1] \times [0,1]$ and $B'' = [0,1] \times [0,100] \times [0,1]$ of two long bricks intersecting in $B' \cap B'' = [0,1] \times [0,1] \times [0,1]$. The integrand is F_{00}, i.e., $\nu_i = \mu_i = 0$ for the exponents in (1.1). The require program input is

Option(1f,22,3c {input:100, 0, 1, 0} *,4,22,3c* {input:1, 0, 100, 0} *,4,22,31).*

The output *Option(l)* shows Q-term with small coefficients. These are typical cancellation effects: The replacement $B''_{k,l}(x,y;X,Y) = Y\left(Q_{k,l}(x,y;Y) - R^-_{k,l}(x,y;X,Y)\right)$ from §5.4 yields several $Q_{k,l}(x,y;Y)$ terms corresponding to $B''_{k,l}(x,y;X,Y)$ with same x-, y-, Y-values but different X-values. Using *Option(6T)* and *Option(6q)* we choose $Tolerance := 1E-5$ and $TolRational := 1E-5$. Then, after *Option(1o),* we get rid of the Q-terms[12].

The numerical evaluation by *Option(5n)* yields the output

value = 181.4393098137807101011276 *** sum of moduli of terms = 8.294779762E+10 .

As discussed in §3.15, this leads to the condition number $8.29_{10}{+}10/181{=}4.6_{10}{+}8$, hence the absolute floating point error is of the size $4.6_{10}{+}8{\times}$eps. Assuming the machine precision eps=2.2_{10}-16 we get 10^{-7} and conclude that 181.43931 should be a correct rounding.

Option(5t) yields the TEX expression (6.14) (after interchanging some terms). We partition this rather long expression into the parts (6.14a) to (6.14i). We will observe that each subexpression has a value comparable with the size of the total result. Therefore, stabilisation considerations can be restricted to each subexpression separately.

First, (6.14a) collects the small and uncritical terms.summing up to $-1.331267\ldots$

More interesting the part (6.14b) involving 6 roots $\sqrt{r}$ with $r \approx 10000$. This sum is discussed in §3.15 and summing up to $-0.41667\ldots$

Similarly, (6.14c) consists of 6 roots $\sqrt{r}$ with $r \approx 20000$. Again, the coefficients sum up to zero: $\frac{32019867}{10} - \frac{48059203}{15} - \frac{97970399}{15} + \frac{98029801}{15} + \frac{10000000}{3} - \frac{33353333}{10} = 0$. Hence, the condition number can be improved as in §3.15. The expression (6.14c) yields the value $-33.712298\ldots$

(6.14d) is a sum of $\ln(r)$ with $r \approx 100$. In this case, the coefficient give the sum -199. The condition number of $\sum a_i \ln(r_i)$ can be improved by rewriting (6.14d) as $(\sum a_i)\ln(100) + \sum a_i \ln(r_i/100)$, since $(\sum a_i)\ln(100) = -199{*}\ln(100) = -916.4\ldots$ is precisely computable, while $\ln(r_i/100) \approx 0.01$ yields a reduced condition number $\sum |a_i \ln(r_i/100)| / |\sum a_i \ln(r_i/100)|$. The true value of (6.14d) is $-996.180\ldots$

(6.14e) is a similar sum of $\ln(r)$ with $r \approx \sqrt{20000} = 141.4\ldots$ Here, the sum of the coefficients is vanishing and (6.14e) equals $111.3967\ldots$

(6.14f) is simpler since this linear combination of $\ln(r)$ with $r \approx 200$ has comparatively small coefficient which add up to $-33 - 66 + \frac{100}{3} + \frac{200}{3} = 1$. (6.14f) has the value $6.293258\ldots$

(6.14g) is the counterpart of (6.14d), since the sum of its coefficients is 199. It is a sum of $\ln(r)$ with $r \approx 100 + \sqrt{20000} = 241.4\ldots$ Its value is $1225.044\ldots$

(6.14h) has the small value $+646800 * \arctan\left(\frac{1}{99\sqrt{9803}}\right) - 666600 * \arctan\left(\frac{1}{100\sqrt{10002}}\right) = -0.666801302\ldots$, although the coefficients do not cancel: $646800 - 666600 = -19800$. Here, the expansion $\arctan x = x - \frac{1}{3}x^3 + O\left(x^4\right)$ for $x \approx 1/10000$ provides accurate results.

(6.14i) is of similar nature. Again the coefficients sum up to -19800. The arguments of arctan are $x \approx 0.0071\ldots$ The value of this subexpression is $-128.987543\ldots$

We observe that an accurate computation of each subproblem reduces the losses by cancellation.

[12] Unfortunately, not all coefficients are represented by rational numbers. The reason is that the ratio $\frac{n}{m}$ requires an integer n larger than the maximal long-integer number. The ratios given in (6.14g) are constructed "by hand" from the floating point numbers.

$$+\frac{1}{10}+\frac{1}{10}*\sqrt{2}-\frac{1}{5}*\sqrt{3}-\frac{5}{3}*\ln\left(\sqrt{2}\right)+\frac{1}{2}*\ln\left(1+\sqrt{2}\right)+\ln\left(1+\sqrt{3}\right)-\frac{2}{3}*\pi \tag{6.14a}$$

$$\begin{aligned}&-\frac{32019867}{5}*\sqrt{9801}+\frac{192060398}{15}*\sqrt{9802}-\frac{96000794}{15}*\sqrt{9803}+\frac{20000000}{3}*\sqrt{10000}\\&-\frac{199940002}{15}*\sqrt{10001}+\frac{33313333}{5}*\sqrt{10002}\end{aligned} \tag{b}$$

$$\begin{aligned}&+\frac{32019867}{10}*\sqrt{19602}-\frac{48059203}{15}*\sqrt{19603}-\frac{97970399}{15}*\sqrt{19801}+\frac{98029801}{15}*\sqrt{19802}\\&+\frac{10000000}{3}*\sqrt{20000}-\frac{33353333}{10}*\sqrt{20001}\end{aligned} \tag{c}$$

$$\begin{aligned}&+\frac{96059601}{2}*\ln\left(\sqrt{9801}\right)-48000398*\ln\left(\sqrt{9802}\right)\\&-50000000*\ln\left(\sqrt{10000}\right)+\frac{99940001}{2}*\ln\left(\sqrt{10001}\right)\\&-32019867*\ln\left(1+\sqrt{9802}\right)+\frac{96000796}{3}*\ln\left(1+\sqrt{9803}\right)\\&+\frac{100000000}{3}*\ln\left(1+\sqrt{10001}\right)-\frac{99940001}{3}*\ln\left(1+\sqrt{10002}\right)\end{aligned} \tag{d}$$

$$\begin{aligned}&-32019867*\ln\left(\sqrt{19602}\right)+\frac{392000399}{6}*\ln\left(\sqrt{19801}\right)-\frac{100000000}{3}*\ln\left(\sqrt{20000}\right)\\&+32019867*\ln\left(1+\sqrt{19603}\right)-\frac{392000399}{6}*\ln\left(1+\sqrt{19802}\right)+\frac{100000000}{3}*\ln\left(1+\sqrt{20001}\right)\end{aligned} \tag{e}$$

$$\begin{aligned}&-33*\ln\left(99+\sqrt{9802}\right)-66*\ln\left(99+\sqrt{9803}\right)\\&+\frac{100}{3}*\ln\left(100+\sqrt{10001}\right)+\frac{200}{3}*\ln\left(100+\sqrt{10002}\right)\end{aligned} \tag{f}$$

$$\begin{aligned}&+\frac{3169966833}{2}*\ln\left(99+\sqrt{19602}\right)-1584013134*\ln\left(99+\sqrt{19603}\right)\\&-1650000000*\ln\left(99+\sqrt{19801}\right)+\frac{3298020033}{2}*\ln\left(99+\sqrt{19802}\right)\\&-1600993350*\ln\left(100+\sqrt{19801}\right)+\frac{4800039800}{3}*\ln\left(100+\sqrt{19802}\right)\\&+\frac{5000\,000000}{3}*\ln\left(100+\sqrt{20000}\right)-\frac{4997000050}{3}*\ln\left(100+\sqrt{20001}\right)\end{aligned} \tag{g}$$

$$+646800*\arctan\left(\frac{1}{99}*\frac{1}{\sqrt{9803}}\right)-666600*\arctan\left(\frac{1}{100}*\frac{1}{\sqrt{10002}}\right) \tag{h}$$

$$\begin{aligned}&-64033200*\arctan\left(\frac{1}{\sqrt{19603}}\right)-66660000*\arctan\left(\frac{1}{\sqrt{20001}}\right)\\&+65993400*\arctan\left(\frac{99}{100}*\frac{1}{\sqrt{19802}}\right)+64680000*\arctan\left(\frac{100}{99}*\frac{1}{\sqrt{19802}}\right).\end{aligned} \tag{i}$$