CALCOLO 40, 33 – 53 (2003)

CALCOLO

On the computation of multi-dimensional single layer harmonic potentials via approximate approximations

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Received: August 2002 / Accepted: November 2002

Abstract. Multidimensional surface potentials associated with elliptic differential operators are defined by surface integrals involving fundamental solutions of the differential operators which become singular when the observation point approaches the surface. Here we combine the choice of basis functions for the so-called approximate approximation of the surface layer density with the integration of the basis functions over the tangential space by the use of appropriate asymptotic expansions. Our approach leads to cubature formulae involving only nodes of a regular grid. These formulae turn out to be extremely efficient provided the saturation error of the approximate approximation is a priori chosen sufficiently small.

1 Introduction

In this paper we describe a new cubature method for the computation of multi-dimensional surface potentials of the form

$$\int_{\Gamma} Q(p-q)\, f(q)\, d\sigma_q ,$$

where Γ is a sufficiently smooth manifold in $\mathbb{R}^d$. It is well-known that, owing to the singularity of the kernel Q at $p = q$, the case in which p is located on or close to the surface Γ requires special attention. This problem is usually addressed by sophisticated methods such as special variable transformations or singularity substraction combined with high order cubature formulae and mesh refinement near to the singularity (see [1,3,5,10,11] and their references).

We propose cubature formulae for these singular or nearly singular integrals which use only the density values at the nodes of a regular grid and the corresponding surface parametrization. The underlying ideas are as follows:

1. The density f is approximated by quasi-interpolation formulae using locally supported smooth radial functions which are centered at regularly distributed nodes on the surface. These approximations were studied in [9] and represent a special case of the so-called *approximate approximations*. Although they do not converge as the grid size tends to zero, it is possible to construct formulae which provide arbitrarily high order approximations up to any prescribed accuracy. Various applications of approximate approximations have already been considered in [4,6–9].
2. The potentials of local basis functions over curved surfaces are approximated by a linear combination of integrals over the tangential space. This approximation is obtained from an asymptotic expansion of the potential by the use of the local parametrization of the surface at the center of the basis function. Again arbitrarily high approximation orders can be achieved by taking the smoothness of the surface into account.
3. Since approximate approximations are very flexible as regards the choice of local basis functions, these are chosen such that the resulting integrals over the $(d-1)$-dimensional tangential space can be transformed to efficiently computable one-dimensional integrals. Thus, the proposed formulae are particularly well-suited for the cubature of integral operators on high-dimensional surfaces.

Since, in principle, both the approximation of the density and the approximation of the potentials can be performed with arbitrarily high order, the proposed cubature formulae can provide very accurate approximations even for moderate grid sizes.

Here we consider this approach for the example of the single layer harmonic potential

$$\begin{aligned} Vf(p) &= \frac{\Gamma(\frac{d-1}{2})}{4(d-2)\pi^{(d-1)/2}} \int\limits_{\Gamma} \frac{f(q)}{|p-q|^{d-2}}\, d\sigma_q \\ &= \omega_d \int\limits_{\Gamma} \frac{f(q)}{|p-q|^{d-2}}\, d\sigma_q . \end{aligned} \tag{1.1}$$

We derive a cubature formula which uses only the values of the normal and of the curvature of Γ at the nodes $\{q_m\}$ of a regular grid. It is proved that this formula approximates the single layer potential uniformly with order $O(h^3|\log h|)$, where h denotes the grid size. It will be clear from the constructions given below, how this approach can be applied to other types of potential operator, and how higher order formulae can be obtained by incorporating more smoothness data about Γ.

The outline of the paper is as follows. In Sect. 2, we describe results on the quasi-interpolation on manifolds by locally supported radial functions, providing estimates for the approximation of the single layer potential (1.1) by linear combinations of surface integrals with small integration domains. In Sect. 3, we approximate these integrals by integrals over the tangential space and obtain uniform error estimates. Here, we also give the cubature formula with weights defined by these $(d-1)$ -dimensional integrals, which can be transformed into one-dimensional ones. This is shown in Sect. 4. Finally, in Sect. 5 we provide numerical results, which are in agreement with the uniform error estimate.

2 Quasi-interpolation on surfaces

After applying a partition of unity we may assume that the function f has compact support on Γ parametrized by $x_d = \varphi(x)$ with a sufficiently smooth function given on a bounded domain $\varphi : \gamma \subset \mathbb{R}^{d-1} \to \mathbb{R}$. Then (1.1) becomes

$$V f(p) = \omega_d \int\limits_{\gamma} \frac{f(y,\varphi(y))}{(|x-y|^2 + (x_d - \varphi(y))^2)^{d/2-1}} \, (1 + |\nabla\varphi(y)|^2)^{1/2} dy \tag{2.1}$$

with $p = (x, x_d)$. To approximate the value of $V f(p)$ we introduce a uniform grid $\{mh \in \gamma \ : m \in \mathbb{Z}^{d-1}\}$ and consider the cubature using the midpoint rule

$$V_h f(p) = \omega_d h^{d-1} \sum_{mh\in\gamma} \frac{f(mh,\varphi(mh))(1 + |\nabla\varphi(mh)|^2)^{1/2}}{(|x-mh|^2 + (x_d - \varphi(mh))^2)^{d/2-1}}. \tag{2.2}$$

Due to the well-known error estimate for the cubature of smooth integrands on uniform grids

$$\left| \int\limits_{\gamma} g(y)\, dy - h^{d-1} \sum_{mh\in\gamma} g(mh) \right| \le c_\ell \, h^\ell \int\limits_{\gamma} |\nabla_\ell g(y)| dy, \ \ \ell = 1, 2, \ldots$$

(see [2]), we have

$$|V f(p) - V_h f(p)| \le c_\ell \, h^\ell (\mathrm{dist}(p, \Gamma))^{1-\ell} \tag{2.3}$$

if $\operatorname{dist}(p,\Gamma) > 0$ for sufficiently smooth f and φ. In the case that $\operatorname{dist}(p,\Gamma)$ is very small, formula (2.2) has to be modified. Usually the cubature of potentials is based on special variable transformations or high order cubature formulae and mesh refinement near to the point p.

To retain the grid and the simple structure of (2.2) we choose a special approximation of the density near the point p. This is a high order quasi-interpolation method applied to an N-times continuously differentiable function f on Γ with compact support, which was studied in [9] and has the form

$$f_h(q) = \mathcal{D}^{-(d-1)/2} \sum_{hm\in\gamma} f(\phi(hm))\, \eta\Big(\frac{q-\phi(hm)}{\sqrt{\mathcal{D}}h\, |\phi'(hm)|^{1/(d-1)}}\Big), \tag{2.4}$$

where, specified to the case considered above, the mapping ϕ is of the form $\phi(x) = (x, \varphi(x))$, and thus $|\phi'(x)| = \sqrt{1+|\nabla\varphi(x)|^2}$.

In formula (2.4), η is chosen as a smooth radial function, i.e., $\eta(x) = \psi(|x|^2/2)$ with a smooth function $\psi : \mathbb{R}^+ \to \mathbb{R}$. Moreover, we assume that η decays rapidly and satisfies the moment conditions

$$\int\limits_{\mathbb{R}^{d-1}} \eta(y)\, dy = 1, \qquad \int\limits_{\mathbb{R}^{d-1}} y^{\boldsymbol{\alpha}}\, \eta(y)\, dy = 0, \tag{2.5}$$

for all multiindices $\boldsymbol{\alpha}$ with $1 \le |\boldsymbol{\alpha}| < N$. Then the following estimates can be proved.

Lemma 2.1 [9] *Assume that the radial function $\eta \in \mathcal{S}(\mathbb{R}^{d-1})$ satisfies the moment conditions* (2.5) *and that $\varphi \in C^{N+1}(\gamma)$. If $f \in C_0^N(\Gamma)$, then for any $\varepsilon > 0$ there exists $\mathcal{D} > 0$ such that, at any point $q \in \Gamma$,*

$$|f_h(q) - f(q)| \le c\, (\sqrt{\mathcal{D}}h)^N\, \|f\|_{C^N(\overline{\Gamma})} + \varepsilon \sum_{k=0}^{N-1} c_k\, (\sqrt{\mathcal{D}}h)^k, \tag{2.6}$$

where c does not depend on f, h and $\mathcal{D}$ and the numbers c_k depend on the values $\partial^{\boldsymbol{\alpha}} f(q)$ for $|\boldsymbol{\alpha}| \le k$.

Remark 1 For any given local basis function η, the functional dependence of ε upon the parameter $\mathcal{D}$ is explicitly known. Therefore, in numerical computations the parameter $\mathcal{D}$ can be chosen so that ε is less than any prescribed accuracy. Then the last term in (2.6), which we call the saturation error because it does not converge to zero, can be neglected and the approximation process and corresponding numerical algorithms behave like Nth order approximations.

Remark 2 Since η is rapidly decaying, the approximation error (2.6) remains valid if the summation in (2.4) is restricted to the grid points $\phi(hm) \in \Gamma$

satisfying

$$|q - \phi(hm)| \leq \sqrt{\mathcal{D}}h \max_{x \in \gamma} |\phi'(x)|^{1/(d-1)} \delta$$

for an appropriately chosen $\delta > 0$.

Here, we use the quasi-interpolant (2.4) of the density to obtain a cubature of the single layer potentials (1.1),

$$V_h f(p) = \frac{\omega_d}{\mathcal{D}^{(d-1)/2}} \sum_{hm \in \gamma} f(\phi(hm)) \times \int_\Gamma \eta\Big(\frac{q - \phi(hm)}{\sqrt{\mathcal{D}}h \, |\phi'(hm)|^{1/(d-1)}}\Big) |p - q|^{2-d} \, d\sigma_q. \tag{2.7}$$

Thus, in suitable norms, the differences $Vf(p) - V_h f(p)$ behave like estimate (2.6). To obtain efficient methods for computing the integrals appearing in the sums over Γ, which in general has a small but curved integration domain, we approximate these by integrals over the tangential space at the points $\phi(hm)$. We are interested in the accuracy of this approximation if, in addition to the first derivatives of ϕ, i.e., the direction of the normal, second derivatives, i.e., the curvatures of Γ, are also used to determine the integrals over the tangential space.

3 Asymptotic formulae for the single layer potential acting on local basis functions

In the following we derive asymptotic formulae of the single layer potential

$$V_h \eta(p) = \omega_d \int_\Gamma |p - q|^{2-d} \, \eta\Big(\frac{q - q_0}{h}\Big) \, d\sigma_q \tag{3.1}$$

as $h \to 0$. Given the normal n to Γ at q_0 we choose a new coordinate system such that q_0 becomes the origin O and the normal coincides with $e_d = (0, \dots, 0, 1)$.

Multiplying by a suitable cut–off function we assume first that η is supported in the ball $B_\delta = \{|p| \leq \delta\}$, $p = (x, x_d) \in \mathbb{R}^d$, $q = (y, y_d) \in \Gamma$. Without loss of generality we can assume that, in a neighborhood U of the origin O, the boundary Γ is given by

$$y_d = \varphi(y) \ \text{ with } \varphi(0) = 0 \ \text{ and } \nabla\varphi(0) = 0. \tag{3.2}$$

We choose h such that $B_{h\delta} \cap \Gamma \subset U$ and write $U_h = \varphi^{-1}(U)$. Then (3.1) takes the form

$$V_h\eta(p) = \omega_d \int_{U_h} (|x-y|^2 + (x_d - \varphi(y))^2)^{1-d/2} \times (1+|\nabla\varphi(y)|^2)^{1/2}\, \eta\Big(\frac{y}{h}, \frac{\varphi(y)}{h}\Big)\, dy. \quad (3.3)$$

First we show that $V_h\eta(p)$ allows an asymptotic expansion in powers of h. Let the parametrization $\varphi(y)$ be a real analytic function and denote the curvature tensor by $K = \|\partial_{jk}\varphi(0)\|_{j,k=1}^{d-1}$. Then, in view of (3.2),

$$\varphi(y) = \frac{1}{2}(Ky, y) + \sum_{|\alpha|\geq 3} \frac{y^\alpha}{\alpha!}\,\partial^\alpha\varphi(0) \quad \text{and}$$
$$|\nabla\varphi(y)|^2 = |Ky|^2 + \sum_{|\alpha|\geq 3} \delta_\alpha y^\alpha. \quad (3.4)$$

Therefore, the area element is, near O, of the form

$$(1+|\nabla\varphi(y)|^2)^{1/2} = 1 + \frac{1}{2}|Ky|^2 + \sum_{k\geq 3} \pi_k(y),$$

where π_k are homogeneous polynomials of degree k. Hence, for $Y = h^{-1}y$ we have

$$ds_y = h^{d-1}\Big(1 + \frac{1}{2}|KY|^2h^2 + \sum_{k\geq 3} h^3\pi_k(Y)\Big)dY.$$

Analogously, if $\eta(y) = \psi(|y|^2/2)$ is real analytic then one obtains from Taylor's expansion

$$\eta\big(\frac{y}{h}, \frac{\varphi(y)}{h}\big) = \sum_{j\geq 0} \frac{(2j-1)!!}{(2j)!}\psi^{(j)}(|Y|^2/2)(h^{-1}\varphi(hY))^{2j}$$
$$= \eta(Y,0) + h^2\frac{(KY,Y)^2}{8}\,\psi'(|Y|^2/2) + \sum_{j\geq 3} h^j p_j(Y, \frac{d}{dt})\,\psi(|Y|^2/2)$$

with certain differential operators $p_j(Y, \frac{d}{dt})$ of order $j/2$ having polynomial coefficients of degree $\leq 2j$. Thus,

$$\eta\big(\frac{y}{h}, \frac{\varphi(y)}{h}\big)(1+|\nabla\varphi(y)|^2)^{1/2}$$
$$= \psi(|Y|^2/2) + \frac{h^2}{8}\Big(4\psi(|Y|^2/2)|KY|^2 + \psi'(|Y|^2/2)(KY,Y)^2\Big) \quad (3.5)$$
$$+ \sum_{j\geq 3} h^j P_j(Y, \frac{d}{dt})\psi(|Y|^2/2)$$

with differential operators $P_j(Y, \frac{d}{dt})$ of order $j/2$ having polynomial coefficients.

Similarly, the kernel function can be expanded in powers of h. We consider two zones, the far field $|p|^2 > 4\delta^2 h^2$ and the near field $|p|^2 < 9\delta^2 h^2$, where the kernel function is singular. In the far field we use the Taylor expansion

$$(|x-y|^2 + (x_d - \varphi(y))^2)^{1-d/2} = \sum_{j\geq 0} \frac{(-\varphi(y))^j}{j!}\, \partial_d^j (|x-y|^2 + x_d^2)^{1-d/2}.$$

Since $|p-q| \geq |p|/2$, we obtain the fact that

$$|\varphi(y)^j||\partial_d^j (|x-y|^2 + x_d^2)^{1-d/2}| \leq \frac{c_j\, |y|^{2j}}{(|x|^2 + x_d^2)^{(d-2+j)/2}} \leq c_j\, h^{2-d+j}.$$

If $|x|^2 + |x_d|^2 < 9\delta^2 h^2$ we expand the kernel with respect to $\varphi(x) - \varphi(y)$:

$$\begin{aligned}(|x-y|^2 &+ (x_d - \varphi(y))^2)^{1-d/2} \\ &= \sum_{j\geq 0} \frac{(\varphi(x)-\varphi(y))^j}{j!} \partial_d^j (|x-y|^2 + (x_d - \varphi(x))^2)^{1-d/2}.\end{aligned}$$

We write $\tilde{x}_d := x_d - \varphi(x)$. Then

$$|(\varphi(x)-\varphi(y))^j|\, |\partial_d^j (|x-y|^2 + \tilde{x}_d^2)^{1-d/2}| \leq \frac{|x-y|^j\, \max|\nabla\varphi|^j}{(|x-y|^2 + \tilde{x}_d^2)^{(d-2+j)/2}},$$

where the maximum of $|\nabla\varphi|$ is taken for $|x| \leq 3\delta h$. Hence,

$$|(\varphi(x)-\varphi(y))^j|\, |\partial_d^j (|x-y|^2 + \tilde{x}_d^2)^{1-d/2}| \leq \frac{c_j\, h^j}{(|x-y|^2 + \tilde{x}_d^2)^{d/2-1}}.$$

Thus $V_h\eta(p)$ can be expanded, at least formally, as a power series with respect to h. The coefficients are given as integral operators over domains in $\mathbb{R}^{d-1}$.

In what follows, we determine the approximations of $V_h\eta(p)$ by using the curvature tensor $K = \|\partial_{jk}\varphi(0)\|_{j,k=1}^{d-1}$ of Γ at O. Due to (3.5), we obtain

$$\Big(1 + \frac{1}{2}|Ky|^2\Big)\, \eta\Big(\frac{y}{h}, \frac{\varphi(y)}{h}\Big) = \sigma\Big(\frac{y}{h}, h\Big) + O(h^3)$$

with the function

$$\begin{aligned}\sigma(y,h) &= \psi(|y|^2/2) \\ &\quad + \frac{h^2}{8}\Big(4\,\psi(|y|^2/2)\,|Ky|^2 + \psi'(|y|^2/2)\,(Ky,y)^2\Big),\end{aligned} \tag{3.6}$$

and we have to analyze the integral

$$\widetilde{V}_h\eta(p) = \omega_d \int\limits_{U_h} (|x-y|^2 + (x_d - \varphi(y))^2)^{1-d/2}\,\sigma(\frac{y}{h},h)\,dy, \qquad (3.7)$$

which differs from the original one by

$$|V_h\eta(p) - \widetilde{V}_h\eta(p)| \le c\,h^3 \int\limits_{U_h} \frac{dy}{(|x-y|^2 + (x_d-\varphi(y))^2)^{d/2-1}}. \qquad (3.8)$$

3.1 Far field $|x|^2 + |x_d|^2 > 4\delta^2 h^2$

Since in this area $|p-q| \ge |p|/2$ we obtain

$$|V_h\eta(p) - \widetilde{V}_h\eta(p)| \le c\,h^{2+d}\,|p|^{2-d}. \qquad (3.9)$$

Then expansion of the kernel gives

$$\frac{1}{(|x-y|^2 + (x_d-\varphi(y))^2)^{d/2-1}} = \frac{1}{(|x-y|^2 + x_d^2)^{d/2-1}} + \frac{(d-2)\,x_d\,\varphi(y)}{(|x-y|^2+x_d^2)^{d/2}} + R_2(p,q)$$

with

$$R_2(p,q) = \int\limits_0^1 (1-t)\mu''(t)dt,$$

where $\mu(t) = \dfrac{1}{(|x-y|^2 + (x_d - t\varphi(y))^2)^{d/2-1}}$.

Note that

$$\mu''(t) = (2-d)\varphi(y)^2\,\frac{|x-y|^2 + (1-d)(x_d - t\varphi(y))^2}{(|x-y|^2 + (x_d - t\varphi(y))^2)^{d/2+1}}$$

and therefore

$$|\mu''(t)| \le \frac{|\varphi(y)|^2}{|p|^d},$$

which, in view of $|y| \le ch$, implies the estimate

$$\left|\omega_d \int\limits_\Gamma R_2(p,q)\,\sigma(\frac{y}{h},h)\,d\sigma_q\right| \le c\,\frac{h^{d+3}}{|p|^d}.$$

Thus, it remains to consider the integrals

$$\omega_d \int\limits_{U_h} \frac{1}{(|x-y|^2+x_d^2)^{d/2-1}}\,\sigma(\frac{y}{h},h)\,dy + \frac{(d-2)\,\omega_d\,x_d}{2}\int\limits_{U_h} \frac{(Ky,y)}{(|x-y|^2+x_d^2)^{d/2}}\,\sigma(\frac{y}{h},h)\,dy + (d-2)\,\omega_d\,x_d \int\limits_{U_h} \frac{\varphi_3(y)}{(|x-y|^2+x_d^2)^{d/2}}\,\sigma(\frac{y}{h},h)\,dy,$$

with $\varphi_3(y)=\sum_{|\alpha|\geq 3}\delta_\alpha y^\alpha$. In the new variables $X=\dfrac{x}{h}$, $X_d=\dfrac{x_d}{h}$, $Y=\dfrac{y}{h}$, the first two integrals transform to

$$\omega_d h\left(\int\limits_{B'_\delta} \frac{\sigma(Y,h)}{(|X-Y|^2+X_d^2)^{d/2-1}}\,dY + \frac{(d-2)\,hX_d}{2}\int\limits_{B'_\delta}\frac{(KY,Y)\,\sigma(Y,h)}{(|X-Y|^2+X_d^2)^{d/2}}\,dY\right),$$

whereas the third integral can be estimated by

$$\left|(d-2)\omega_d x_d \int\limits_{U_h} \frac{\varphi_3(y)}{(|x-y|^2+x_d^2)^{d/2}}\sigma\Big(\frac{y}{h},h\Big)dy\right| \leq c h^{d+2}|p|^{1-d}. \quad (3.10)$$

Here $B'_\delta = B_\delta \cap \mathbb{R}^{d-1}$ denotes the support of the radial function η in $\mathbb{R}^{d-1}$. From (3.6) we therefore obtain as an approximation to $V_h\eta(p)$ in the far field

$$\begin{aligned}&\omega_d h\int\limits_{B'_\delta}\frac{\psi(|Y|^2/2)}{(|X-Y|^2+X_d^2)^{d/2-1}}\,dY\\ &+\frac{\omega_d\,(d-2)h^2X_d}{2}\int\limits_{B'_\delta}\frac{(KY,Y)\,\psi(|Y|^2/2)}{(|X-Y|^2+X_d^2)^{d/2}}\,dY\\ &+\frac{\omega_d h^3}{8}\int\limits_{B'_\delta}\frac{4\,|KY|^2\,\psi(|Y|^2/2)+(KY,Y)^2\,\psi'(|Y|^2/2)}{(|X-Y|^2+X_d^2)^{d/2-1}}\,dY,\end{aligned} \quad (3.11)$$

which in the following is denoted by $\widehat{V}_h\eta(p)$ and, in view of (3.9), provides uniform approximations of $V_h\eta(p)$ of order $h^{d+2}|p|^{1-d}$. Note that the third integral in formula (3.11) is of order $O(h^{d+1}|p|^{2-d})$, which, for $|p|=O(h)$, is the same as for the error term (3.10).

3.2 Near field $|x|^2 + |x_d|^2 < 9\delta^2 h^2$

Here (3.8) leads to

$$|V_h\eta(p) - \widetilde{V}_h\eta(p)| \le c\,h^3 \int\limits_{U_h} \frac{dy}{|x-y|^{d-2}} \le c\,h^4. \tag{3.12}$$

As mentioned above, we use the Taylor expansion of the kernel about the point $(x-y, \tilde{x}_d)$, where $\tilde{x}_d = x_d - \varphi(x)$. From (3.6) we obtain the integrals

$$\omega_d \int\limits_{U_h} \frac{1}{(|x-y|^2+\tilde{x}_d^2)^{d/2-1}}\,\sigma(\frac{y}{h},h)\,dy = \omega_d h \int\limits_{B'_\delta} \frac{\psi(|Y|^2/2)\,dy}{(|X-hY|^2+\widetilde{X}_d^2)^{d/2-1}}$$
$$+\frac{\omega_d\,h^3}{8}\int\limits_{B'_\delta} \frac{4|KY|^2\psi(|Y|^2/2)+(KY,Y)^2\psi'(|Y|^2/2)}{(|X-hY|^2+\widetilde{X}_d^2)^{d/2-1}}\,dY,$$

where $X = h^{-1}x$, $\widetilde{X}_d = h^{-1}(x_d - \varphi(x))$. The succeeding term in Taylor's expansion gives

$$\omega_d(d-2)\,\tilde{x}_d \int\limits_{U_h} \frac{\varphi(y)-\varphi(x)}{(|x-y|^2+\tilde{x}_d^2)^{d/2}}\sigma(\frac{y}{h},h)\,dy.$$

If we replace $\varphi(y)$ by (Ky, y), the error satisfies

$$\left|\omega_d(d-2)\,\tilde{x}_d \int\limits_{U_h} \frac{\varphi_3(y)-\varphi_3(x)}{(|x-y|^2+\tilde{x}_d^2)^{d/2}}\sigma(\frac{y}{h},h)\,dy\right|$$
$$\le c \int\limits_{U_h} \frac{(|y|^2+|x|^2)\,dy}{(|x-y|^2+\tilde{x}_d^2)^{d/2-1}} = O(h^3).$$

Thus, for points $p = (hX, hX_d)$ in the near field, we obtain the formula

$$\widehat{V}_h\eta(p) = \omega_d h \int\limits_{B'_\delta} \frac{\psi(|Y|^2/2)}{(|X-Y|^2+\widetilde{X}_d^2)^{d/2-1}}\,dY$$
$$+\frac{\omega_d(d-2)h^2\,\widetilde{X}_d}{2}\int\limits_{B'_\delta} \frac{((KY,Y)-(KX,X))\,\psi(|Y|^2/2)}{(|X-Y|^2+\widetilde{X}_d^2)^{d/2}}\,dY, \tag{3.13}$$

which in view of (3.12) provides uniform approximations of $V_h\eta(p)$ of order h^3.

Thus the single layer potential of the Laplacian is approximated for all $p \in \mathbb{R}^d$ by (3.11) and (3.13) with the uniform error $O(h^{d+2}/(|p|+h)^{d-1})$.

3.3 Matching in the area $2\delta h \le |p| \le 3\delta h$

According to the remark at the end of Sect. 3.1 we have to show that the sum of the first two integrals in (3.11) differs from (3.13) by higher order terms if the point $p = (hX, hX_d)$ lies in the matching area. Since $X_d = \widetilde{X}_d + \varphi(x)/h$ and $(|X - Y|^2 + X_d^2)^{1-d/2}$ is smooth for $q = (hY, y_d) \in U_h$ we have

$$\begin{aligned}\frac{1}{(|X-Y|^2 + X_d^2)^{d/2-1}} &= \frac{1}{(|X-Y|^2 + \widetilde{X}_d^2)^{d/2-1}} \\ &\quad - \frac{\omega_d (d-2)\varphi(hX)\widetilde{X}_d}{h(|X-Y|^2 + \widetilde{X}_d^2)^{-d/2}} + O\Big(\frac{\varphi(hX)^2}{h^2}\Big).\end{aligned} \tag{3.14}$$

Thus, if we replace $\varphi(hX)$ by $h^2(KX, X)/2$ in (3.14), we see that formula (3.11) differs from (3.13) by terms of order $O(h^3)$, i.e., in the overlapping region both formulae generate the same asymptotic error.

3.4 Approximation error

The approximation of $V_h f(p)$ is now given by

$$\widetilde{V}_h f(p) = \mathcal{D}^{(1-d)/2} \sum_{hm \in \gamma} f(\phi(hm)) \widehat{V}_{h_m} \eta(p - \phi(hm)), \tag{3.15}$$

where the parameter $h_m = \sqrt{\mathcal{D}}h\, |\phi'(hm)|^{1/(d-1)}$ and the formulae for $\widehat{V}_{h_m}\eta$ are determined by (3.11) or (3.13) in dependence on the value of $|p - \phi(hm)|$. Due to the uniform error estimate, the difference $|V_h \eta(p) - \widehat{V}_h \eta(p)|$ can be estimated by

$$\begin{aligned}&\frac{\omega_d}{\mathcal{D}^{(d-1)/2}} \sum_{hm\in\gamma} |f(\phi(hm))| \frac{(\sqrt{\mathcal{D}}h\, |\phi'(hm)|^{1/(d-1)})^{d+2}}{(|p - \phi(hm)| + \sqrt{\mathcal{D}}h\, |\phi'(hm)|^{1/(d-1)})^{d-1}} \\ &\le c(\sqrt{\mathcal{D}}h)^3 \int_\gamma |f((\phi(y))| \frac{|\phi'(y)|^{(d+2)/(d-1)}}{(|p - \phi(y)| + \sqrt{\mathcal{D}}h\, |\phi'(y)|^{1/(d-1)})^{d-1}}\, dy \\ &\le c(\sqrt{\mathcal{D}}h)^3 \int_\Gamma \frac{|f(q)|}{(|p-q| + \sqrt{\mathcal{D}}h)^{d-1}}\, d\sigma_q \\ &\le c\|f\|_{C(\overline{\Gamma})} (\sqrt{\mathcal{D}}h)^3 |\log(\max(\sqrt{\mathcal{D}}h, \mathrm{dist}(p, \Gamma)))|.\end{aligned} \tag{3.16}$$

Note that the integrals appearing in the formulae (3.11) or (3.13) are restricted to the domain B'_δ, which is the support of the basis function η in $\mathbb{R}^{d-1}$ after multiplication by a suitable cut–off function. Due to the rapid decay of η one can obviously extend the integration domain to the whole of $\mathbb{R}^{d-1}$ giving an error less than a prescribed tolerance ε.

Thus, we fix $\delta' > 0$ such that

$$\int\limits_{\mathbb{R}^{d-1}\setminus B_{\delta'}} |y|^2 |\eta(y)|\, dy \le \varepsilon,$$

with ε the saturation error from Lemma 2.1. To compute the approximation of (1.1) we choose a local coordinate system with origin at the point $\phi(hm)$ such that the x_d-axis is directed as the normal to Γ at this point. In the new coordinate system, the surface Γ is given locally by the mapping $x_d = \varphi(x)$, $x \in \mathbb{R}^{d-1}$. The corresponding curvature tensor we denote by $K = \|\partial_{jk}\varphi(0)\|_{j,k=1}^{d-1}$. Let $p - \phi(hm) = (x, x_d) = (hX, hX_d)$, and consider the approximations of $V_h\eta(p - \phi(hm))$:

1. if $|p - \phi(hm)| \ge h\delta'$, then

$$\begin{aligned}\widehat{V}_h\eta(p-\phi(hm)) &= \omega_d h \int\limits_{\mathbb{R}^{d-1}} \frac{\psi(|Y|^2/2)}{(|X-Y|^2+X_d^2)^{d/2-1}}\, dY \\ &+ \frac{\omega_d\,(d-2)h^2 X_d}{2} \int\limits_{\mathbb{R}^{d-1}} \frac{(KY,Y)\,\psi(|Y|^2/2)}{(|X-Y|^2+X_d^2)^{d/2}}\, dY \\ &+ \frac{\omega_d h^3}{8} \int\limits_{\mathbb{R}^{d-1}} \frac{4\,|KY|^2\,\psi(|Y|^2/2) + (KY,Y)^2\,\psi'(|Y|^2/2)}{(|X-Y|^2+X_d^2)^{d/2-1}}\, dY;\end{aligned} \tag{3.17}$$

2. if $|p - \phi(hm)| < h\delta'$, then

$$\begin{aligned}\widehat{V}_h\eta(p-\phi(hm)) &= \omega_d h \int\limits_{\mathbb{R}^{d-1}} \frac{\psi(|Y|^2/2)}{(|X-Y|^2+\widetilde{X}_d^2)^{d/2-1}}\, dY \\ &+ \frac{\omega_d(d-2)h^2\,\widetilde{X}_d}{2} \int\limits_{\mathbb{R}^{d-1}} \frac{((KY,Y)-(KX,X))\,\psi(|Y|^2/2)}{(|X-Y|^2+\widetilde{X}_d^2)^{d/2}}\, dY,\end{aligned} \tag{3.18}$$

where $\widetilde{X}_d = X_d - h^{-1}\varphi(hX)$. Then from Lemma 2.1 and (3.16) we derive

Theorem 3.1 *Suppose that the radial function $\eta \in \mathcal{S}(\mathbb{R}^d)$ satisfies the moment condition* (2.5) *with $N = 4$. Then the single layer potential*

$$Vf(p) = \omega_d \int\limits_{\Gamma} \frac{f(q)}{|p-q|^{d-2}}\, d\sigma_q$$

is approximated by the sum (3.15) *with order*

$$|Vf(p) - \widetilde{V}_h f(p)| = O((\sqrt{\mathcal{D}}h)^3 |\log(\max(\sqrt{\mathcal{D}}h, \operatorname{dist}(p,\Gamma)))| + \varepsilon), \tag{3.19}$$

provided that the surface Γ *has* C^4*-smoothness and* $f \in C_0^3(\Gamma)$. *The saturation term* ε *can be made negligibly small if* $\mathcal{D}$ *is sufficiently large.*

3.5 Cubature formula

As mentioned above we use formulae (3.17) only if $|p - \phi(hm)|$ is small, otherwise we can use the simple midpoint rule (2.2). To give the corresponding bounds for $|p - \phi(hm)|$ we introduce a cut–off function χ_h with the property that $\chi_h(q) = 1$ for $|q| \le h^\beta$ and $\chi_h(q) = 0$ for $|q| \ge (h^\beta + h^{1/4})$ for some $\beta \in (0, 1)$ to be specified later. We split the single layer potential into two integrals

$$\omega_d \int\limits_\Gamma \frac{f(q)\chi_h(p-q)}{|p-q|^{d-2}}\, d\sigma_q + \omega_d \int\limits_\Gamma \frac{f(q)(1-\chi_h(p-q))}{|p-q|^{d-2}}\, d\sigma_q \qquad (3.20)$$

and apply Theorem 3.1 to the first one. Note, that $f(q)\chi_h(p - q) \neq 0$, $q \in \Gamma$, only for $\mathrm{dist}(p, \Gamma) < (h^\beta + h^{1/4})$. Since $|\nabla \chi_h| \le ch^{-1/4}$, we have

$$\|f\,\chi_h(p-\cdot)\|_{C^4(\overline{\Gamma})} \le ch^{-1}\|f\|_{C^4(\overline{\Gamma})}.$$

Thus, in view of Theorem 2.1, the function $f(q)\chi_h(p-q)$ can be approximated on Γ by the quasi-interpolant

$$\mathcal{D}^{-(d-1)/2} \sum_{|p-\phi(hm)|<h^{\beta-1/4}} f(\phi(hm)) \times \chi_h(p-\phi(hm))\, \eta\Big(\frac{q-\phi(hm)}{\sqrt{\mathcal{D}}h\,|\phi'(hm)|^{1/(d-1)}}\Big) \qquad (3.21)$$

with error

$$c\,(\sqrt{\mathcal{D}}h)^3\,\|f\|_{C^4(\overline{\Gamma})} + \varepsilon \sum_{k=0}^{3} c_k\,(\sqrt{\mathcal{D}}h)^{3k/4}.$$

Consequently, if $f \in C_0^4(\Gamma)$, then we can argue as in Theorem 3.1 to derive the estimate

$$\Big|\omega_d \int\limits_\Gamma \frac{f(q)\chi_h(p-q)}{|p-q|^{d-2}}\, d\sigma_q - \mathcal{D}^{(1-d)/2} \sum_{|p-\phi(hm)|<h^\beta+h^{1/4}} f(\phi(hm))\chi_h(p-\phi(hm))\widetilde{V}_{h_m}\eta(p-\phi(hm))\Big| = O((\sqrt{\mathcal{D}}h)^3|\log(\sqrt{\mathcal{D}}h)| + \varepsilon).$$

Thus, it remains to choose β such that the second integral in (3.20) is approximated with order $O(h^3)$ by

$$h^{d-1}\omega_d \sum_{mh\in\gamma} \frac{f(\phi(mh))(1-\chi_h(p-\phi(mh)))}{|p-\phi(mh)|^{d-2}}|\phi'(mh)|.$$

If $\operatorname{dist}(p,\Gamma) \geq h^\beta + h^{1/4}$, then $\chi_h(p-\phi(y)) = 0$ and

$$\begin{aligned}
&\int_\gamma \left|\nabla_\ell\left(\frac{f(\phi(y))}{|p-\phi(y)|^{d-2}}\sqrt{1+|\nabla\varphi(y)|^2}\right)\right| dy \\
&\quad \leq \sum_{j=0}^{\ell} c_j \left|\nabla_{\ell-j}(f(\phi(y))\sqrt{1+|\nabla\varphi(y)|^2})\right| \int_\gamma \frac{dy}{|p-\phi(y)|^{d+j-2}} \\
&\quad \leq \sum_{j=0}^{\ell} c_j \left|\nabla_{\ell-j}(f(\phi(y))\sqrt{1+|\nabla\varphi(y)|^2})\right| \int_0^{\operatorname{diam}\gamma} \frac{r^{d-2}\,dr}{|r+h^\beta+h^{1/4}|^{d+j-2}}.
\end{aligned}$$

Thus,

$$h^\ell \int_\gamma \left|\nabla_\ell\left(\frac{f(\phi(y))}{|p-\phi(y)|^{d-2}}\sqrt{1+|\nabla\varphi(y)|^2}\right)\right| dy \leq c\,h^\ell(h^\beta+h^{1/4})^{1-\ell}.$$

If $\operatorname{dist}(p,\Gamma) < h^\beta + h^{1/4}$, we have

$$\left|\nabla_{\ell-j}\left(f(\phi(y))(1-\chi_h(p-\phi(y)))\sqrt{1+|\nabla\varphi(y)|^2}\right)\right| \leq ch^{(j-\ell)/4},$$

and

$$\int_{|p-\phi(y)|\geq h^\beta} \frac{dy}{|p-\phi(y)|^{d+j-2}} \leq c\,h^{\beta(1-j)}$$

so that

$$h^\ell \int_\gamma \left|\nabla_\ell\left(\frac{f(\phi(y))(1-\chi_h(p-\phi(y)))}{|p-\phi(y)|^{d-2}}\sqrt{1+|\nabla\varphi(y)|^2}\right)\right| dy \leq c\,h^{\ell(1-\beta)}h^\beta.$$

Hence, depending on the smoothness $f \in C_0^\ell(\Gamma)$ with $\ell \geq 4$, the value $\beta = 1 - 2/(\ell-1)$ provides the following estimate of the cubature error:

$$\begin{aligned}
&\left|\omega_d \int_\Gamma \frac{f(q)(1-\chi_h(p-q))}{|p-q|^{d-2}}\,d\sigma_q \right. \\
&\left. - h^{d-1}\omega_d \sum_{mh\in\gamma} \frac{f(\phi(mh))(1-\chi_h(p-\phi(mh)))}{|p-\phi(mh)|^{d-2}}|\phi'(mh)|\right| \\
&\quad \leq ch^3\|f\|_{C^\ell(\overline{\Gamma})}.
\end{aligned}$$

Therefore Theorem 3.1 remains valid if, for instance, $f \in C_0^5(\Gamma)$, and $\chi_h(q)$ is chosen such that $\chi_h(q) = 1$ for $|q| \le h^{1/2}$ and $\chi_h(q) = 0$ for $|q| \le h^{1/2} + h^{1/4}$. Then formulae (3.17) are applied in the region $h\delta' \le |p - \phi(hm)| \le (h^{1/2} + h^{1/4})\delta'$ with the function values $f(hm)\chi_h(p - hm)$, and the midpoint rule with the values $f(hm)(1 - \chi_h(p - hm))$ is applied in the region $|p - \phi(hm)| \ge h^{1/2}\delta'$.

Summarizing, we obtain the following result.

Theorem 3.2 *Suppose that the surface* Γ *is* $C^{\ell+1}$, $f \in C_0^{\ell}(\Gamma)$, $\ell \ge 4$, *and set* $\beta = 1 - 2/(\ell - 1)$. *Then the single layer potential*

$$Vf(p) = \omega_d \int\limits_{\Gamma} \frac{f(q)}{|p - q|^{d-2}}\, d\sigma_q$$

is approximated by the sum of

$$\mathcal{D}^{(1-d)/2} \sum_{|p-\phi(hm)|<h^{\beta}+h^{1/4}} f(\phi(hm))\chi_h(p - \phi(hm))\widetilde{V}_{h_m}(p - \phi(hm))$$

and

$$h^{d-1}\omega_d \sum_{|p-\phi(hm)|>h^{\beta}} \frac{f(\phi(mh))(1 - \chi_h(p - \phi(mh)))}{|p - \phi(mh)|^{d-2}} |\phi'(mh)|$$

with order (3.19). *Here* $\chi_h(q)$ *is a sufficiently smooth cut–off function in* $\mathbb{R}^d$ *vanishing outside the ball* $|q| > h^{\beta} + h^{1/4}$ *and equal to* 1 *for* $|q| < h^{\beta}$. *The saturation term* ε *can be made negligibly small if* $\mathcal{D}$ *is sufficiently large.*

4 Basis functions

Here we show that the integrals appearing in formulae (3.17) and (3.18) can be converted into one-dimensional integrals. Thus, the proposed integration procedure for surface integration is also well-suited for high-dimensional cases. Since the basis function η is radial, one can use the well-known formula for the convolution of radial functions. The $(d - 1)$-dimensional Fourier transform of a radial function $\eta(y) = \psi(|y|^2/2)$ is itself radial and can be obtained from the formula

$$\mathcal{F}\eta(|\lambda|) = \frac{2\pi}{|\lambda|^{(d-3)/2}} \int\limits_0^{\infty} \psi(r^2/2) J_{(d-3)/2}(2\pi|\lambda|r)\, r^{(d-1)/2}\, dr \qquad (4.1)$$

where J_n is the Bessel function of the first kind of order n. Therefore the convolution of η with a radial kernel $Q(x) = Q(|x|)$ has the form

$$\int\limits_{\mathbb{R}^{d-1}} Q(x-y)\eta(y)\,dy = \frac{2\pi}{|x|^{(d-3)/2}} \int\limits_0^\infty \mathcal{F}Q(r)\,\mathcal{F}\eta(r)\,r^{(d-1)/2}\,J_{(d-3)/2}(2\pi r|x|)\,dr. \quad (4.2)$$

In the following we give explicit formulae for the integrals approximating the single and double layer potentials, if the Gaussian function $\eta(x) = (2\pi)^{(1-d)/2}e^{-|x|^2/2}$ is chosen as the local basis function.

In order to obtain one-dimensional integrals if the Gaussian is used as local basis function, consider the integral

$$\frac{1}{(2\pi)^{(d-1)/2}} \int\limits_{\mathbb{R}^{d-1}} Q(|x-y|)\,e^{-|y|^2/2}\,dy = \frac{1}{(2\pi)^{(d-1)/2}} \int\limits_{\mathbb{R}^{d-1}} Q(|y|)\,e^{-|x-y|^2/2}\,dy$$
$$= \frac{e^{-|x|^2/2}}{(2\pi)^{(d-1)/2}} \int\limits_0^\infty Q(r)\,e^{-r^2/2}r^{d-2}\,dr \int\limits_{S^{d-2}} e^{|x|r\cos\theta}d\omega,$$

where S^{d-2} is the unit sphere in $\mathbb{R}^{d-1}$. From the basic relation for (4.1),

$$\int\limits_{S^{d-2}} e^{ia\cos\theta}d\omega = \frac{(2\pi)^{(d-1)/2}}{a^{(d-3)/2}} J_{(d-3)/2}(a),$$

we obtain

$$\int\limits_{S^{d-2}} e^{|x|r\cos\theta}d\omega = \frac{(2\pi)^{(d-1)/2}\,J_{(d-3)/2}(i|x|r)}{(i|x|r)^{(d-3)/2}} = \frac{(2\pi)^{(d-1)/2}\,I_{(d-3)/2}(|x|r)}{(|x|r)^{(d-3)/2}}$$

with the modified Bessel function of the first kind I_n. Hence, even if the Fourier transform of the kernel Q is not available, the $(d-1)$-dimensional convolution with the Gaussian function can be computed from a one-dimensional integral given by

$$\frac{1}{(2\pi)^{(d-1)/2}} \int\limits_{\mathbb{R}^{d-1}} Q(|x-y|)\,e^{-|y|^2/2}\,dy = \frac{e^{-|x|^2/2}}{|x|^{(d-3)/2}} \int\limits_0^\infty Q(r)\,e^{-r^2/2}r^{(d-1)/2}\,I_{(d-3)/2}(|x|r)\,dr.$$

Note that the Gaussian satisfies the moment conditions (2.5) only for $N = 2$. To achieve the higher order for the quasi-interpolants as required in Theorem 3.1, one can choose, for example, linear combinations of Gaussians. In the numerical tests we used the function

$$\eta(x) = \frac{2e^{-|x|^2}}{\pi^{(d-1)/2}} - \frac{e^{-|x|^2/2}}{(2\pi)^{(d-1)/2}}$$

which satisfies (2.5) for $N = 4$.

Next, we give the formulae based on (4.2) for the integrals appearing in (3.17) and (3.18) with $\psi(y) = e^{-y}$. Since

$$\omega_d \int\limits_{\mathbb{R}^{d-1}} \frac{e^{-2\pi i(x,\lambda)}}{(|x|^2 + x_d^2)^{d/2-1}}\,dx = \frac{\Gamma(\frac{d-1}{2})}{8\sqrt{\pi}\,\Gamma(\frac{d}{2})}\,\frac{e^{-2\pi|\lambda||x_d|}}{|\lambda|},$$

formula (4.2) yields

$$\begin{aligned} \mathcal{I}_0(x, x_d) &= \omega_d \int\limits_{\mathbb{R}^{d-1}} \frac{e^{-|y|^2/2}}{(|x-y|^2 + x_d^2)^{d/2-1}}\,dy \\ &= \frac{2^{(d-3)/2}\pi^{d/2}}{|x|^{(d-3)/2}}\,\frac{\Gamma(\frac{d-1}{2})}{\Gamma(\frac{d}{2})} \\ &\quad \times \int\limits_0^\infty e^{-2\pi r(\pi r + |x_d|)}\, r^{(d-3)/2}\, J_{(d-3)/2}(2\pi r|x|)\,dr. \end{aligned} \tag{4.3}$$

Then we consider the integral

$$\mathcal{I}_1(x, x_d) = \omega_d\,(d-2)x_d \int\limits_{\mathbb{R}^{d-1}} \frac{(Ky, y)\,e^{-|y|^2/2}}{(|x-y|^2 + x_d^2)^{d/2}}\,dy.$$

Obviously

$$(Ky, y)\,e^{-|y|^2/2} = ((K\nabla, \nabla) + \mathrm{tr}K)e^{-|y|^2/2},$$

where $\nabla = (\partial_1, \ldots, \partial_{d-1})$ and $\mathrm{tr}K = \Delta\varphi(0)$, and hence

$$\mathcal{I}_1(x, x_d) = \omega_d\,(d-2)((K\nabla, \nabla) + \mathrm{tr}K) \int\limits_{\mathbb{R}^{d-1}} \frac{x_d e^{-|y|^2/2}}{(|x-y|^2 + x_d^2)^{d/2}}\,dy.$$

Since

$$\int\limits_{\mathbb{R}^{d-1}} \frac{x_d\, e^{-2\pi i(x,\lambda)}}{(|x|^2 + x_d^2)^{d/2}}\,dx = \frac{\pi^{d/2}\mathrm{sign}(x_d)\,e^{-2\pi|\lambda||x_d|}}{\Gamma(\frac{d}{2})}$$

with sign(0) = 0, we finally derive

$$\mathcal{I}_1(x, x_d) = 2^{(d-3)/2}\pi^{(d+2)/2}\,\mathrm{sign}(x_d)\,\frac{\Gamma(\frac{d-1}{2})}{\Gamma(\frac{d}{2})}$$
$$\times((K\nabla,\nabla)+\mathrm{tr}K)\int_0^\infty e^{-2\pi r(\pi r+|x_d|)}\,r^{(d-1)/2}\,\frac{J_{(d-3)/2}(2\pi r|x|)}{|x|^{(d-3)/2}}\,dr.$$

The series expansion

$$J_n(2\pi r|x|) = (\pi r|x|)^n\sum_{j=0}^\infty\frac{(-1)^j(\pi r|x|)^{2j}}{j!\,\Gamma(j+n+1)}$$

shows that the function

$$(K\nabla,\nabla)\,\frac{J_{(d-3)/2}(2\pi r|x|)}{|x|^{(d-3)/2}} \tag{4.4}$$

is smooth. Consider a radial function $g(|x|)$ and write $\omega = x/|x|$. Then

$$(K\nabla,\nabla)g(|x|) = (K\omega,\omega)\Big(g''(|x|)-\frac{g'(|x|)}{|x|}\Big)+\mathrm{tr}K\,\frac{g'(|x|)}{|x|}.$$

Therefore (4.4) can be expressed by using the values of $(K\omega,\omega)$, $\mathrm{tr}K$ and either trigonometric functions (d even) or the Bessel functions J_0 and J_1 (d odd) . For example, if $d = 3$, then

$$(K\nabla,\nabla)J_0(2\pi r|x|)$$
$$= 4\pi r(K\omega,\omega)\Big(\pi r J_0(2\pi r|x|)-\frac{J_1(2\pi r|x|)}{|x|}\Big)+2\pi r\,\mathrm{tr}K\,\frac{J_1(2\pi r|x|)}{|x|},$$

whereas, for $d = 4$,

$$(K\nabla,\nabla)\,\frac{J_{1/2}(2\pi r|x|)}{|x|^{1/2}} = (K\nabla,\nabla)\,\frac{\sin(2\pi r|x|)}{\pi r^{1/2}|x|}$$
$$= \mathrm{tr}K\,\frac{2\pi|x|r\cos(2\pi r|x|)-\sin(2\pi r|x|)}{\pi r^{1/2}|x|^3}$$
$$-(K\omega,\omega)\,\frac{(4\pi^2r^2|x|^2-3)\sin(2\pi r|x|)+6\pi r|x|\cos(2\pi r|x|)}{\pi r^{1/2}|x|^3}.$$

Lastly consider the integral

$$\omega_d\int_{\mathbb{R}^{d-1}}\frac{(4\,|Ky|^2-(Ky,y)^2)e^{-|y|^2/2}}{(|x-y|^2+x_d^2)^{d/2-1}}\,dy$$

appearing in formula (3.17). It is easy to see that

$$\begin{aligned}&\big(4\,|Ky|^2-(Ky,y)^2\big)e^{-|y|^2/2}\\ &\quad=\Big(-(K\nabla,\nabla)^2-2|K\nabla|^2+(\mathrm{tr}K)^2-2\det K\,(\Delta+2)\Big)e^{-|y|^2/2};\end{aligned}$$

therefore one has to determine

$$\Big(-(K\nabla,\nabla)^2-2|K\nabla|^2+(\mathrm{tr}K)^2-2\det K\,(\Delta+2)\Big)\frac{J_{(d-3)/2}(2\pi r|x|)}{|x|^{(d-3)/2}}.$$

For the radial function $g(|x|)$ we get

$$\begin{aligned}&\Big(-(K\nabla,\nabla)^2-2|K\nabla|^2+(\mathrm{tr}K)^2-2\det K\,(\Delta+2)\Big)g(|x|)\\
&=(K\omega,\omega)^2\Big(-g^{(4)}(|x|)+6\frac{g^{(3)}(|x|)}{|x|}-15\frac{g''(|x|)}{|x|^2}+15\frac{g'(|x|)}{|x|^3}\Big)\\
&\quad+|K\omega|^2\Big(-4\frac{g^{(3)}(|x|)}{|x|}+12\frac{g''(|x|)}{|x|^2}-12\frac{g'(|x|)}{|x|^3}-2g''(|x|)+2\frac{g'(|x|)}{|x|}\Big)\\
&\quad+\mathrm{tr}K\,(K\omega,\omega)\Big(-2\frac{g^{(3)}(|x|)}{|x|}+6\frac{g''(|x|)}{|x|^2}-6\frac{g'(|x|)}{|x|^3}\Big)\\
&\quad+(\mathrm{tr}K)^2\Big(-3\frac{g''(|x|)}{|x|^2}+3\frac{g'(|x|)}{|x|^3}-2\frac{g'(|x|)}{|x|}+g(|x|)\Big)\\
&\quad+\det K\Big(4\frac{g''(|x|)}{|x|^2}-4\frac{g'(|x|)}{|x|^3}-2g''(|x|)+2\frac{g'(|x|)}{|x|}-4g(|x|)\Big).\end{aligned}$$

The differential expressions can easily be calculated by the use of programs like Maple or Mathematica.

5 Numerical examples

The approach presented was tested numerically in the computation of single layer potentials for the three-dimensional Laplacian. We applied the combined formulae to obtain the integral

$$\frac{1}{4\pi}\int_\Gamma \frac{e^{-|q|^2}}{|p-q|}\,d\sigma_q, \tag{5.1}$$

for a paraboloid Γ given by $x_3 = k_{11}x_1^2 + 2k_{12}x_1x_2 + k_{11}x_2^2$. Using the quasi-interpolation formula (3.21) with the local function

$$\eta(q)=\frac{2e^{-|q|^2}}{\pi^{(d-1)/2}}-\frac{e^{-|q|^2/2}}{(2\pi)^{(d-1)/2}},$$

Table 5.1. Approximation order for the flat surface

dist(p, Γ)	$h = 0.4$	$h = 0.2$	$h = 0.1$	$h = 0.05$
2.0	12.5505	12.4669	7.4823	0.0000
0.1	3.6585	3.9123	3.8671	3.9177
0.01	3.7009	4.0864	3.9906	3.8467
0.001	3.7054	4.2484	3.8495	3.8415
0.0001	3.7071	4.3752	3.7439	3.8589
0.00001	3.3292	3.7139	3.8543	3.9662
0.0	3.3262	3.6974	4.0360	3.8644

Table 5.2. Approximation order for the paraboloid

dist(p, Γ)	$h = 0.4$	$h = 0.2$	$h = 0.1$	$h = 0.05$
2.0	4.0356	17.9653	1.8432	0.0002
0.1	3.4212	3.0952	2.9031	2.9200
0.01	3.3849	3.2257	3.0537	2.7146
0.001	3.1082	2.5078	2.8485	2.9774
0.0001	3.1773	2.8232	3.1836	2.8206
0.00001	2.8018	2.5479	3.0889	2.8765
0.0	4.8512	3.0970	2.6406	2.8437

the approximation error of the density $e^{-|q|^2}$ is $O((\sqrt{\mathcal{D}}h)^4 + \varepsilon)$. The same rate is shown for the cubature of the potential for flat Γ, i.e., $k_{ij} = 0$. In Table 5.1, we give the approximation order obtained by halving the step size h for a randomly chosen point p with prescribed distance from Γ. We chose the parameter $\mathcal{D} = 3.0$ in formula (2.4) in order to keep the saturation error less than 10^{-10}. The high orders for dist$(p, \Gamma) = 2.0$ result from the fact that the simple midpoint is used for all mesh points. In the other cases we approximate the density by a fourth order quasi-interpolant. Since Γ is flat, formulae (3.17) and (3.18) provide the exact values of the potentials of the basis functions. Therefore the single layer potential is approximated with the same order as the density.

In Table 5.2, we provide the results for the curved surface $x_3 = x_1^2 + 2x_1x_2 + 2x_2^2$, which are in total agreement with the assertion of Theorem 3.2.

Acknowledgements. This work was carried out while the first author was visiting the University of Stuttgart as an Alexander von Humboldt Research Award winner, and was supported in part by the Collaborative Research Center "Multifield Problems in Continuum Mechanics" (Sonderforschungsbereich Mehrfeldprobleme in der Kontinuumsmechanik, SFB 404) at the University of Stuttgart.

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