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Accurate Computation of Multi-Dimensional Riesz Potentials

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The paper discusses a fast method for computing the Riesz potentials in the framework of the method approximate approximations. By combining high-order cubature formulas with tensor product approximations, we derive an approximation of the potentials which is fast, accurate and provides approximation formulas of high order. The action of volume potentials on the basis functions introduced in the theory of approximate approximations allows one-dimensional integral representations with separable integrands, i.e. a product of functions depending on only one of the variables. Then a separated representation of the density, combined with a suitable quadrature rule, leads to a tensor product representation of the integral operator. Since only one-dimensional operations are used, the resulting method is effective also in the high-dimensional case.

Keywords: Multidimensional convolution, Riesz potential, separated representation, approximate approximations.

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1. Introduction

The Riesz potential is known to be defined as

$$\mathcal{R}_\alpha(f) = \frac{1}{\gamma_n(\alpha)} \int_{\mathbb{R}^n} \frac{f(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{n-\alpha}} d\mathbf{y}, \qquad 0<\alpha<n \tag{1.1}$$

where the normalizing constant is given by the relation

$$\gamma_n(\alpha) = \frac{\pi^{n/2} 2^\alpha \Gamma\left(\frac{\alpha}{2}\right)}{\Gamma\left(\frac{n-\alpha}{2}\right)}.$$

The function f is called the density of the potential $\mathcal{R}_\alpha$. The Riesz potential is strictly related to the fractional Laplace operator $(-\Delta)^{\alpha/2}, \alpha \in (0,2)$ in $\mathbb{R}^n$, also known as the Riesz fractional derivative. Namely,

$$(-\Delta)^{\alpha/2} \mathcal{R}_\alpha f = f, \qquad 0<\alpha<n,$$

(cf., e.g., [24], [26]). The fractional Laplacian appears in different fields of mathematics (PDE, harmonic analysis, semigroup theory, probabilistic theory, cf., e.g.,

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[4], [8], [9] and the references therein) as well as in many applications (optimization, finance, materials science, water waves, cf., e.g., [21], [5], [6], [23] and the references therein).

It is well known that, due to the singularity of the integral (1.1), usual cubature methods are very time consuming and often exceed the capacity of available computer systems. In this paper, we propose a method of an arbitrary high order for the approximation of $\mathcal{R}_\alpha f$ which is based on the approximation of the function f via the basis functions introduced in the theory approximate approximations (cf. [20] and the references therein), which are product of Gaussians and special polynomials. Then the n-dimensional convolution (1.1) applied to the basis functions is represented through a one-dimensional integral where the integrand has a separated representation, i.e., it is a product of functions depending only on one of the variables.

An accurate quadrature rule and a separated representation of the density f provide a separated representation for $\mathcal{R}_\alpha f$. Thus, only one-dimensional operations are used and the resulting approximation procedure is fast and effective also in high-dimensional cases, and provides approximations of high order, up to a small saturation error.

The concept of approximate approximations and first related results were introduced by V. Mazya in [17], [18]. Various aspects of a general theory of these approximations were further developed and formulas of various integral and pseudo-differential operators have been obtained (cf. [20] and the review paper [25]). By combining cubature formulas for volume potentials based on approximate approximations with the strategy of separated representations (cf., e.g., [3], [7]), it is possible to derive a method for approximating volume potentials which is accurate and fast also in the multidimensional case and provides approximation formulas of high order. This procedure was applied successfully for the fast integration of the harmonic [10], biharmonic [14], diffraction [13], elastic and hydrodynamic [15] potentials. In [11], [12] this approach was extended to parabolic problems. The method described in this paper has been obtained in [16] and applied for the fast approximation of the fractional Laplacian.

The outline of the paper is the following. In Section 2, we describe the method and provide error estimates. In Section 3 we derive the one-dimensional integral representations of the Riesz potential applied to our basis functions. In Section 4, for densities f with a separated representation, we derive tensor product representations for $\mathcal{R}_\alpha f$ which admit efficient one-dimensional operations. Finally, we report on numerical results, illustrating that our formulas are accurate and provide the predicted approximation rates $2, 4, 6, 8$ in dimension $n = 3$ and also if the dimension is high ($n = 10^k, k = 1, 2, 3, 4$).

2. Description of the method

Approximate quasi-interpolants have the following form

$$\mathcal{M}_{h,\mathcal{D}} f(\mathbf{x}) := \mathcal{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right) \tag{2.1}$$

with fixed positive parameters h and $\mathcal{D}$ and with some generating function η sufficiently smooth and of rapid decay such that η satisfies suitable moment conditions (see (2.3)). Then the sum

$$\mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}}f)(\mathbf{x}) = \frac{(h\sqrt{\mathcal{D}})^\alpha}{\mathcal{D}^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m})\mathcal{R}_\alpha(\eta)\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right) \tag{2.2}$$

provides an approximation formula for (1.1), provided $\mathcal{R}_\alpha(\eta)$ can be computed analytically or at least efficiently. Due to the semi-analytic cubature nature of the formula (2.2), the fractional gradient $\nabla^{\alpha-1}f = -\nabla\mathcal{R}_{2-\alpha}f$ and the fractional Laplacian $(-\Delta)^{\alpha/2}f = -\Delta\mathcal{R}_{2-\alpha}f$ can be approximated by $-\nabla\mathcal{R}_{2-\alpha}(\mathcal{M}_{h,\mathcal{D}}f)$ and $-\Delta\mathcal{R}_{2-\alpha}(\mathcal{M}_{h,\mathcal{D}}f)$, respectively. Hence, from (2.2) we deduce approximation formulas for the fractional gradient and the fractional Laplacian (cf. [16]).

We denote by $\mathcal{S}(\mathbb{R}^n)$ the Schwartz space of smooth and rapidly decaying functions and by $W_p^N(\mathbb{R}^n)$, $N \in \mathbf{N}$, the Sobolev space of the $L_p(\mathbb{R}^n)$ functions whose generalized derivatives up to the order N also belong to $L_p(\mathbb{R}^n)$. In the following, $\nabla_k f$ denotes the vector of partial derivatives $\{\partial^\beta f\}_{|\beta|=k}$. The norm in $W_p^N(\mathbb{R}^n)$ is defined by

$$||f||_{W_p^N} = \sum_{k=0}^{N} ||\nabla_k f||_{L_p}, \qquad ||\nabla_k f||_{L_p} = \sum_{|\beta|=k} ||\partial^\beta f||_{L_p}.$$

If $\eta \in \mathcal{S}(\mathbb{R}^n)$ satisfies the moment condition of order N,

$$\int_{\mathbb{R}^n} \eta(\mathbf{x})\, \mathbf{x}^\alpha d\mathbf{x} = \delta_{0,\alpha}, \quad 0 \le |\alpha| < N, \tag{2.3}$$

then for any $f \in W_\infty^N(\mathbb{R}^n)$ the approximation error of the quasi-interpolation can be estimated pointwise by

$$|f(\mathbf{x}) - \mathcal{M}_{h,\mathcal{D}}f(\mathbf{x})| \le c_\eta(\sqrt{\mathcal{D}}h)^N \|\nabla_N f\|_{L_\infty} + \sum_{k=0}^{N-1} \varepsilon_k(\mathcal{D})(\sqrt{\mathcal{D}}h)^k \big|\nabla_k f(\mathbf{x})\big|$$

with

$$0 < \varepsilon_k(\mathcal{D}) \le \sum_{\mathbf{m}\in\mathbb{Z}^n\setminus\{0\}} \big|\nabla_k \mathcal{F}\eta(\sqrt{\mathcal{D}}\mathbf{m})\big|,$$

$$\lim_{\mathcal{D}\to\infty} \sum_{\mathbf{m}\in\mathbb{Z}^n\setminus\{0\}} \big|\nabla_k \mathcal{F}\eta(\sqrt{\mathcal{D}}\mathbf{m})\big| = 0$$

([20, p.34]). Similar approximation properties in integral norms are valid. The following theorem was proved in [20, p.42].

Theorem 2.1: *Suppose that* $\eta \in \mathcal{S}(\mathbb{R}^n)$ *satisfies* (2.3). *Then for any* $f \in W_p^L(\mathbb{R}^n)$, $1 \le p \le \infty$ *and* $L > n/p$, $L \ge N$, *the quasi-interpolant* (2.1) *satis-*

fies

$$||f - \mathcal{M}_{h,\mathcal{D}} f||_{L_p} \le c_\eta (\sqrt{\mathcal{D}} h)^N ||\nabla_N f||_{L_p} + \sum_{k=0}^{N-1} \frac{\varepsilon_k(\mathcal{D})}{(2\pi)^k} (\sqrt{\mathcal{D}} h)^k ||\nabla_k f||_{L_p}$$

where the constant c_η does not depend on f, h and $\mathcal{D}$.

Let us estimate the approximation error of the cubature formula (2.2) for the Riesz potential $\mathcal{R}_\alpha f$. By construction, the cubature error equals to

$$\mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}} f) - \mathcal{R}_\alpha f = \mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}} f - f).$$

From Sobolev's theorem, the operator $\mathcal{R}_\alpha$ is a bounded mapping from $L_p(\mathbb{R}^n)$ into $L_q(\mathbb{R}^n)$, $1 < p < n/\alpha$, $1/q = 1/p - \alpha/n$ ([26, p.119]). Then,

$$||\mathcal{R}_\alpha f - \mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}} f)||_{L_q} \le A_{pq}^{(\alpha)} ||f - \mathcal{M}_{h,\mathcal{D}} f||_{L_p} \tag{2.4}$$

where $A_{pq}^{(\alpha)}$ denotes the norm of $\mathcal{R}_\alpha : L_p(\mathbb{R}^n) \to L_q(\mathbb{R}^n)$. Theorem 2.1 and (2.4) immediately give the following error estimate.

Theorem 2.2: *Suppose that $\eta \in \mathcal{S}(\mathbb{R}^n)$ satisfies* (2.3)*. Let $n \ge 3$, $0 < \alpha < 2$, $1 < p < n/\alpha$, $1/q = 1/p - \alpha/n$ and let $f \in W_p^L(\mathbb{R}^n)$ with $L > n/p$, $L \ge N$. Then*

$$\begin{aligned} &||\mathcal{R}_\alpha f - \mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}} f)||_{L_q} \\ &\qquad \le A_{pq}^{(\alpha)} \left(c_\eta (\sqrt{\mathcal{D}} h)^N ||\nabla_N f||_{L_p} + \sum_{k=0}^{N-1} \frac{\varepsilon_k(\mathcal{D})}{(2\pi)^k} (\sqrt{\mathcal{D}} h)^k ||\nabla_k f||_{L_p} \right). \end{aligned}$$

The previous theorem shows that if the function η and the parameter $\mathcal{D}$ are chosen such that the values $\varepsilon_k(\mathcal{D})$ are sufficiently small, then the cubature of $\mathcal{R}_\alpha$ approximates with order h^N up to the prescribed accuracy. However, by the smoothing properties of $\mathcal{R}_\alpha$ ([26, p.131]), also the saturation error converges to zero with rate h^α. Indeed, quasi-interpolation has the remarkable property that it converges in certain weak norms since the saturation error, which is caused by fast oscillating functions, converges weakly to zero. We denote by

$$\mathcal{F} f(\mathbf{x}) = \int_{\mathbb{R}^n} f(\mathbf{y}) \mathrm{e}^{2\pi i \mathbf{x} \cdot \mathbf{y}} d\mathbf{y}$$

the Fourier transform of f and by $\mathcal{F}^{-1}$ its inverse. Let $H_p^s(\mathbb{R}^n)$ be the Bessel potential space, equipped with the norm

$$||f||_{H_p^s} = ||\mathcal{F}^{-1}((1 + 4\pi^2 |\cdot|^2)^{s/2} \mathcal{F} f)||_{L_p} = ||(I - \Delta)^{s/2} f||_{L_p}$$

(cf., e.g., [26, p.130], [19, p.516]). Instead of Theorem 2.1 we use the following result, a direct consequence of [20, Theorem 4.6].

Theorem 2.3: *Suppose that $\eta \in \mathcal{S}(\mathbb{R}^n)$ satisfies* (2.3)*. For any $\varepsilon > 0$, there exists $\mathcal{D} > 0$ such that for any $f \in H_p^L(\mathbb{R}^n)$, $1 < p < \infty$, $L > n/p$, $L \ge N \ge 2$ and*

$\alpha \in (0,2)$, *the quasi-interpolant* (2.1) *satisfies*

$$||f - \mathcal{M}_{h,\mathcal{D}} f||_{H_p^{-\alpha}} \leq c_\eta (h\sqrt{\mathcal{D}})^N ||f||_{H_p^L} + \varepsilon h^\alpha c_{p,\alpha} \sum_{k=0}^{N-1-[\alpha]} \frac{(\sqrt{\mathcal{D}}h)^k}{k!} ||\nabla_k f||_{H_p^\alpha}$$

where $[\alpha]$ *denotes the integer part of* α*, the constants* c_η *and* $c_{p,\alpha}$ *do not depend on* f*,* h *and* $\mathcal{D}$*.*

We can formulate the following.

Theorem 2.4: *Suppose that* $\eta \in \mathcal{S}(\mathbb{R}^n)$ *satisfies* (2.3). *Let* $0 < \alpha < 2$, $1 < p < n/\alpha$, $1/q = 1/p - \alpha/n$. *For any* $f \in W_p^L(\mathbb{R}^n)$ *with* $L \geq N \geq 2$ *and* $L > n/p$*, there exist positive constants* $C, C_{p,\alpha}, C_{q,\alpha}$ *not depending on* f*,* h *and* $\mathcal{D}$ *such that*

$$||\mathcal{R}_\alpha f - \mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}} f)||_{L_q} \leq C(h\sqrt{\mathcal{D}})^N ||f||_{W_p^L} +$$
$$\varepsilon h^\alpha \sum_{k=0}^{N-1-[\alpha]} \frac{(h\sqrt{\mathcal{D}})^k}{k!} \left(C_{p,\alpha} A_{p,q}^{(\alpha)} ||\nabla_k f||_{H_p^\alpha} + C_{q,\alpha} ||\nabla_k f||_{H_q^\alpha} \right).$$

Proof: We have ([26, p.117])

$$\begin{aligned} ||\mathcal{R}_\alpha f||_{L_q} &= ||(-\Delta)^{-\alpha/2}(I-\Delta)^{-\alpha/2}(I-\Delta)^{\alpha/2} f)||_{L_q} \\ &= ||(-\Delta)^{-\alpha/2}(I-\Delta)^{-\alpha/2} f||_{H_q^\alpha}. \end{aligned}$$

The norm $||u||_{H_q^\alpha}$ is equivalent to $||u||_{L_q} + ||(-\Delta)^{\alpha/2} u||_{L_q}$ ([24, Theorem 7.16]). Hence, keeping in mind (2.4), we deduce

$$\begin{aligned} ||\mathcal{R}_\alpha f||_{L_q} &\leq c_1(|||\mathcal{R}_\alpha (I-\Delta)^{-\alpha/2} f||_{L_q} + ||(I-\Delta)^{-\alpha/2} f||_{L_q}) \\ &\leq c_1(A_{pq}^{(\alpha)} ||(I-\Delta)^{-\alpha/2} f|||_{L_p} + ||(I-\Delta)^{-\alpha/2} f||_{L_q}) \\ &= c_1(A_{pq}^{(\alpha)} ||f - \mathcal{M}_{h,\mathcal{D}} f||_{H_p^{-\alpha}} + ||f - \mathcal{M}_{h,\mathcal{D}} f||_{H_q^{-\alpha}}). \end{aligned}$$

We use Theorem 2.3, the fact that $H_p^s(\mathbb{R}^n)$ are interpolation spaces that coincide with the Sobolev spaces for $s \in \mathbf{N}$, $H_p^s(\mathbb{R}^n) = W_p^s(\mathbb{R}^n)$([19, p. 458]) and the continuous embedding $W_p^L(\mathbb{R}^n) \subset W_q^{L-2}(\mathbb{R}^n)$ ([2, p.97]) to obtain the required estimate. □

After having estimated the cubature error, to construct high order cubature formulas for (1.1) it remains to choose η which satisfies the moment condition (2.3), such that the values $\varepsilon_k(\mathcal{D})$ can be made arbitrarily small by a proper choice of $\mathcal{D}$ and the integral $\mathcal{R}_\alpha \eta$ can be computed analytically or at least efficiently. If the integral $\mathcal{R}_\alpha \eta$ is expressed analytically then (2.2) is a semi-analytic cubature formula: by simple differentiation of (2.2) one obtains immediately approximations of the corresponding derivative of (1.1).

3. One-dimensional integral representations

For second order approximations we choose $\eta_2(\mathbf{x}) = \pi^{-n/2}\mathrm{e}^{-|\mathbf{x}|^2}$. It satisfies (2.3) with $N = 2$. The convolution of the Gaussian with a radial function can be obtained from the following formula proved in [20, (5.15)]

$$\int_{\mathbb{R}^n} Q(|\mathbf{x}-\mathbf{y}|)\mathrm{e}^{-|\mathbf{y}|^2} d\mathbf{y} = \frac{2\pi^{n/2}\mathrm{e}^{-|\mathbf{x}|^2}}{|\mathbf{x}|^{n/2-1}} \int_0^\infty Q(r) I_{n/2-1}(2|\mathbf{x}|r) r^{n/2} \mathrm{e}^{-r^2} dr$$

with the modified Bessel function of the first kind I_s ([1, p.374]). In our case we get

$$\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{2\pi^{n/2}\mathrm{e}^{-|\mathbf{x}|^2}}{\gamma_n(\alpha)|\mathbf{x}|^{n/2-1}} \int_0^\infty r^{\alpha-n/2}\mathrm{e}^{-r^2} I_{n/2-1}(2|\mathbf{x}|r) dr. \tag{3.1}$$

The integrand in the last integral is summable in $(0, +\infty)$ because $\alpha \in (0, 2)$, $I_{n/2-1}(r) \approx \frac{r^{n/2-1}}{2\Gamma(n/2)}$, $r \to 0^+$ ([1, 9.6.7]) and $I_{n/2-1}(r) \approx \frac{\mathrm{e}^r}{\sqrt{2\pi}\sqrt{r}}$, $r \to \infty$ ([1, 9.7.1]).

The one-dimensional integral in (3.1) can be expressed by means of the confluent hypergeometric functions ${}_1F_1$ ([22, 2.15.5.4])

$$\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{\Gamma(\frac{n-\alpha}{2})}{2^\alpha\Gamma(\frac{n}{2})} \mathrm{e}^{-|\mathbf{x}|^2} {}_1F_1(\frac{\alpha}{2}, \frac{n}{2}, |\mathbf{x}|^2)\,. \tag{3.2}$$

By using Kummer transformation ([1, 13.1.27]) we can also write

$$\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{\Gamma(\frac{n-\alpha}{2})}{2^\alpha\Gamma(\frac{n}{2})} {}_1F_1(\frac{n-\alpha}{2}, \frac{n}{2}, -|\mathbf{x}|^2). \tag{3.3}$$

The formula (2.2) together with (3.2) gives rise to second order semi-analytic cubature formulas for $\mathcal{R}_\alpha$ up to the saturation error.

The second order cubature formula for the approximation of $\mathcal{R}_\alpha$ on the uniform grid $\{h\mathbf{k}\}$ leads to the convolutional sum

$$\mathcal{R}_\alpha(\mathcal{M}_{h,\mathcal{D}} f)(h\mathbf{k}) = \frac{(h\sqrt{\mathcal{D}})^\alpha}{(\pi\mathcal{D})^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})\left(\frac{\mathbf{k}-\mathbf{m}}{\sqrt{\mathcal{D}}}\right). \tag{3.4}$$

The computation of the multidimensional convolutional sum (3.4), even for the space dimension $n = 3$, is very time consuming and often exceed the capacity of available computer systems. We propose a method which reduces the computational effort and gives rise to fast formulas. We write (3.2) in a different way by using the integral representation of the hypergeometric functions ${}_1F_1$ ([1, 13.2.1])

$${}_1F_1(a, c, z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 \mathrm{e}^{z\tau} \tau^{a-1}(1-\tau)^{-a+c-1} d\tau, \quad \mathrm{Re}\,(c) > \mathrm{Re}\,(a) > 0\,.$$

With the substitution $\tau = t/(1+t)$ we get

$$ {}_1F_1(a,c,z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^\infty \mathrm{e}^{\frac{t}{1+t}z} \frac{t^{a-1}}{(1+t)^c} dt, \quad \mathrm{Re}\,(c) > \mathrm{Re}\,(a) > 0\,. $$

Hence, from (3.2) we obtain

$$ \Phi_2(\mathbf{x}) := \mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})(\mathbf{x}) = \frac{1}{2^\alpha \Gamma(\frac{\alpha}{2})} \int_0^\infty \frac{t^{-1+\frac{\alpha}{2}} \mathrm{e}^{-\frac{|\mathbf{x}|^2}{1+t}}}{(1+t)^{n/2}} dt. \tag{3.5} $$

The representation of Φ_2 in (3.5) is very advantageous because the integrand is expressed by elementary functions and it has a separated representation. Then a separated representation of Φ_2 is obtained by applying an accurate quadrature rule with nodes $\{\tau_s\}$ and weights $\{\omega_s\}$:

$$ \Phi_2\left(\frac{\mathbf{k}-\mathbf{m}}{\sqrt{\mathcal{D}}}\right) \approx \frac{\pi^{-n/2}}{2^\alpha \Gamma(\frac{\alpha}{2})} \sum_s \omega_s \frac{\tau_s^{-1+\frac{\alpha}{2}}}{(1+\tau_s)^{n/2}} \mathrm{e}^{-\frac{|\mathbf{k}-\mathbf{m}|^2}{\mathcal{D}(1+\tau_s)}}. \tag{3.6} $$

The computation of the sum in (3.4) with $\mathcal{R}_\alpha \eta_2 = \Phi_2$ in (3.6) is very efficient for densities that allow a separated representation, i.e., for given accuracy ε, they can be represented as a sum of products of vectors in dimension 1

$$ f(\mathbf{x}) = \sum_{p=1}^{P} \prod_{j=1}^{n} f_j^{(p)}(x_j) + \mathcal{O}(\epsilon), \qquad \mathbf{x} = (x_1, ..., x_n). \tag{3.7} $$

We infer that an approximation of $\mathcal{R}_\alpha f(h\mathbf{k})$ can be computed by the sum of products of one-dimensional convolutions

$$ (\mathcal{R}_\alpha f)(h\mathbf{k}) \approx \frac{1}{(\pi\mathcal{D})^{n/2}} \frac{(h\sqrt{\mathcal{D}})^\alpha}{2^\alpha \Gamma(\frac{\alpha}{2})} \prod_{p=1}^{P} \sum_s \frac{\omega_s \tau_s^{-1+\frac{\alpha}{2}}}{(1+\tau_s)^{n/2}} \prod_{j=1}^{n} \sum_{m_j \in \mathbb{Z}} f_j^{(p)}(hm_j) \mathrm{e}^{-\frac{(k_j-m_j)^2}{\mathcal{D}(1+\tau_s)}}. $$

To derive high order approximation formulas, we assume as basis functions the tensor product of univariate functions

$$ \eta_{2M}(\mathbf{x}) = \prod_{j=1}^{n} \widetilde{\eta}_{2M}(x_j); \quad \widetilde{\eta}_{2M}(x_j) = \frac{(-1)^{M-1}}{2^{2M-1}\sqrt{\pi}\,(M-1)!} \frac{H_{2M-1}(x_j)\mathrm{e}^{-x_j^2}}{x_j} \tag{3.8} $$

where H_k are the Hermite polynomials

$$ H_k(x) = (-1)^k \mathrm{e}^{x^2} \left(\frac{d}{dx}\right)^k \mathrm{e}^{-x^2}. $$

The function η_{2M} satisfies the moment conditions of order $2M$ and the values

$\varepsilon_k(\mathcal{D}) = \mathcal{O}(P_k(\sqrt{\mathcal{D}})\mathrm{e}^{-\pi^2\mathcal{D}})$ ([20, Theorem 3.5]). Then (3.8) gives rise to approximation formulas of order $2M$ plus the saturation error.

We provide one-dimensional integral representations for $\mathcal{R}_\alpha\eta_{2M}$ similar to that obtained in (3.5). Using the relation ([20, p.55])

$$\widetilde{\eta}_{2M}(x) = \frac{1}{\sqrt{\pi}} \sum_{s=0}^{M-1} \frac{(-1)^s}{s!4^s} \frac{d^{2s}}{dx^{2s}} \mathrm{e}^{-x^2},$$

integrating by parts and making use of (3.5), we get

$$\begin{aligned}
\mathcal{R}_\alpha(\eta_{2M})(\mathbf{x}) &= \frac{1}{\gamma_n(\alpha)\pi^{n/2}} \prod_{j=1}^{n} \sum_{s_j=0}^{M-1} \frac{(-1)^{s_j}}{s_j!4^{s_j}} \frac{d^{2s_j}}{dx_j^{2s_j}} \int\limits_{\mathbb{R}^n} \frac{\mathrm{e}^{-|\mathbf{y}|^2}}{|\mathbf{x}-\mathbf{y}|^{n-\alpha}} d\mathbf{y} \\
&= \frac{1}{\pi^{n/2}} \prod_{j=1}^{n} \sum_{s_j=0}^{M-1} \frac{(-1)^{s_j}}{s_j!4^{s_j}} \frac{d^{2s_j}}{dx_j^{2s_j}} (\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2}))(\mathbf{x}) \\
&= \frac{\pi^{-n/2}}{2^\alpha\Gamma(\frac{\alpha}{2})} \prod_{j=1}^{n} \sum_{s_j=0}^{M-1} \frac{(-1)^{s_j}}{s_j!4^{s_j}} \frac{d^{2s_j}}{dx_j^{2s_j}} \int\limits_0^\infty \frac{t^{-1+\frac{\alpha}{2}} \mathrm{e}^{-\frac{|\mathbf{x}|^2}{1+t}}}{(1+t)^{n/2}} dt\,.
\end{aligned}$$

Due to the relation

$$\frac{d^{2s}}{dx^{2s}} \mathrm{e}^{-ax^2} = a^s H_{2s}(\sqrt{a}x)\mathrm{e}^{-ax^2}, \qquad a > 0, \quad s \geq 0,$$

we obtain the following one-dimensional integral representation with separated integrand for $\mathcal{R}_\alpha(\eta_{2M})$

$$\Phi_{2M}(\mathbf{x}) := \mathcal{R}_\alpha(\eta_{2M})(\mathbf{x}) = \frac{\pi^{-n/2}}{2^\alpha\Gamma(\frac{\alpha}{2})} \int\limits_0^\infty \prod_{j=1}^{n} S_M(\frac{1}{t+1}, x_j) \frac{\mathrm{e}^{-\frac{x_j^2}{1+t}}}{(1+t)^{1/2}}\, t^{-1+\frac{\alpha}{2}} dt, \quad (3.9)$$

where we introduced the polynomials in x

$$S_M(a,x) = \sum_{s=0}^{M-1} \frac{(-1)^s a^s}{s!4^s} H_{2s}(\sqrt{a}x), \quad a > 0.$$

For example, we have

$$\begin{aligned}
S_1(a,x) &= 1 \\
S_2(a,x) &= 1 + \frac{a}{2} - a^2x^2; \\
S_3(a,x) &= S_2(a,x) + \frac{a^2}{8}\left(4a^2x^4 - 12ax^2 + 3\right); \\
S_4(a,x) &= S_3(a,x) + \frac{a^3}{48}\left(-8a^3x^6 + 60a^2x^4 - 90ax^2 + 15\right).
\end{aligned}$$

4. Implementation and numerical results

From representations (2.2),(3.9), we derive the approximating formula

$$\mathcal{R}_\alpha f(\mathbf{x}) \approx \mathcal{R}_{\alpha,h}^{(M)} f(\mathbf{x}) := \frac{(h\sqrt{\mathcal{D}})^\alpha}{\mathcal{D}^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m})\Phi_{2M}\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right). \tag{4.1}$$

The computation of (4.1) on a uniform grid $h\mathbf{k} = (hk_1, ..., hk_n)$ leads to discrete convolutions

$$\mathcal{R}_\alpha f(h\mathbf{k}) \approx \mathcal{R}_{\alpha,h}^{(M)} f(h\mathbf{k}) = \frac{(h\sqrt{\mathcal{D}})^\alpha}{\mathcal{D}^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) a_{\mathbf{k}-\mathbf{m}}^{(M)}, \tag{4.2}$$

where

$$a_{\mathbf{k}}^{(M)} = \frac{\pi^{-n/2}}{2^\alpha \Gamma(\frac{\alpha}{2})} \int_0^\infty \prod_{j=1}^n S_M(\frac{1}{t+1}, k_j) \frac{\mathrm{e}^{-\frac{k_j^2}{1+t}}}{(1+t)^{1/2}}\, t^{-1+\frac{\alpha}{2}} dt.$$

For functions f with a separated representation (3.7), by applying an accurate quadrature rule, we derive the approximation of the convolutional sum in (4.2) via separated representations.

It is known that the double exponential formulas for numerical integration, proposed by Takahasi and Mori ([27], see also [28]), are highly efficient. The idea is to transform a given integral to an integral over the real line through a change of variable $t = \phi(u)$ such that the integrand has a double exponential decay, and then apply the trapezoidal formula to the transformed integral. For the transformation function $\phi(u)$, we make the substitution proposed in [27]

$$t = \phi(u) \text{ with } \phi(u) = \mathrm{e}^{\psi(u)}, \quad \psi(u) = a(b(u - \mathrm{e}^{-u}) + \mathrm{e}^{b(u-\mathrm{e}^{-u})})$$

with positive constants a and b. After the substitution we have

$$a_{\mathbf{k}}^{(M)} = \frac{\pi^{-n/2}}{2^\alpha \Gamma(\frac{\alpha}{2})} \int_{-\infty}^\infty \prod_{j=1}^n S_M(\frac{1}{\phi(u)+1}, k_j) \frac{\mathrm{e}^{-\frac{k_j^2}{1+\phi(u)}}}{(1+\phi(u))^{1/2}} (\phi(u))^{\frac{\alpha}{2}} \psi'(u) du\,.$$

The quadrature with the trapezoidal rule with step size τ gives

$$a_{\mathbf{k}}^{(M)} = \frac{\tau\pi^{-n/2}}{2^\alpha \Gamma(\frac{\alpha}{2})} \sum_s \prod_{j=1}^n S_M(\frac{1}{\phi(s\tau)+1}, k_j) \frac{\mathrm{e}^{-\frac{k_j^2}{1+\phi(s\tau)}}}{(1+\phi(s\tau))^{1/2}} (\phi(s\tau))^{\frac{\alpha}{2}} \psi'(s\tau)\,.$$

In the remainder of the paper, we provide results of some experiments which show the accuracy and the convergence orders of the method. The sum $\mathcal{R}_{\alpha,h}^{(M)} f$ in (4.1) approximates $\mathcal{R}_\alpha f$ with order $\mathcal{O}(h^{2M} + h^\alpha \mathrm{e}^{-\pi^2\mathcal{D}})$. Therefore, if $\mathcal{D}$ is large enough, then $\mathcal{R}_{\alpha,h}^{(M)} f$ behaves in numerical computations like a high-order formula. We compute the volume potential $\mathcal{R}_\alpha$ of $f(\mathbf{x}) = \mathrm{e}^{-|\mathbf{x}|^2}$ which has the exact value in (3.2)

Table 1. Absolute errors, relative errors, and approximation rates for the 3-dimensional volume potential $\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})$ at (.6, .6, .6) using $\mathcal{R}^{(M)}_{\alpha,h}(\mathrm{e}^{-|\cdot|^2})$, with $\alpha = 1.5$.

	$M=4$			$M=3$		
h^{-1}	absolute error	relative error	rate	absolute error	relative error	rate
10	0.137D-06	0.454D-06		0.214D-05	0.709D-05	
20	0.620D-09	0.205D-08	7.79	0.386D-07	0.128D-06	5.79
40	0.251D-11	0.832D-11	7.95	0.625D-09	0.207D-08	5.95
80	0.977D-14	0.324D-13	8.01	0.986D-11	0.327D-10	5.99
160	0.278D-15	0.920D-15	5.14	0.154D-12	0.509D-12	6.00

	$M=2$			$M=1$		
h^{-1}	absolute error	relative error	rate	absolute error	relative error	rate
10	0.123D-04	0.409D-04		0.484D-02	0.160D-01	
20	0.556D-06	0.184D-05	4.47	0.122D-02	0.404D-02	1.99
40	0.311D-07	0.103D-06	4.16	0.305D-03	0.101D-02	2.00
80	0.188D-08	0.624D-08	4.04	0.763D-04	0.253D-03	2.00
160	0.117D-09	0.387D-09	4.00	0.191D-04	0.632D-04	2.00

Table 2. Absolute errors, relative errors and approximation rates for the 3-dimensional volume potential $\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})$ at $(1,1,1)$ using $\mathcal{R}^{(M)}_{\alpha,h}(\mathrm{e}^{-|\cdot|^2})$, with $\alpha = 0.5$.

	$M=4$			$M=3$		
h^{-1}	absolute error	relative error	rate	absolute error	relative error	rate
10	0.146D-06	0.173D-05		0.502D-05	0.594D-04	
20	0.602D-09	0.714D-08	7.92	0.837D-07	0.991D-06	5.91
40	0.238D-11	0.283D-10	7.98	0.133D-08	0.157D-07	5.98
80	0.930D-14	0.110D-12	8.00	0.208D-10	0.247D-09	5.99
160	0.971D-16	0.115D-14	6.58	0.326D-12	0.386D-11	6.00

	$M=2$			$M=1$		
h^{-1}	absolute error	relative error	rate	absolute error	relative error	rate
10	0.134D-04	0.158D-03		0.182D-03	0.215D-02	
20	0.883D-06	0.105D-04	3.92	0.473D-04	0.560D-03	1.94
40	0.560D-07	0.663D-06	3.98	0.119D-04	0.141D-03	1.99
80	0.351D-08	0.416D-07	3.99	0.299D-05	0.354D-04	2.00
160	0.220D-09	0.260D-08	4.00	0.748D-06	0.886D-05	2.00

(or (3.3)), by using the approximating formulas (4.1). In Tables 1-2 we report on absolute errors, relative errors and the approximation rates

$$(\log|\mathcal{R}_\alpha f(\mathbf{x}) - \mathcal{R}^{(M)}_{\alpha,2h} f(\mathbf{x})| - \log|\mathcal{R}_\alpha f(\mathbf{x}) - \mathcal{R}^{(M)}_{\alpha,h} f(\mathbf{x})|)/\log 2$$

for the computations of the 3-dimensional volume potential $\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})$ at a fixed point by assuming $\alpha = 1.5$ (Table 1) and $\alpha = 0.5$ (Table 2). The numerical results confirm the h^{2M} convergence of the approximating formula when $M = 1, 2, 3, 4$. For small h, the 8th-order formula reaches the saturation error.

Table 3 shows that the method is effective also for higher space dimensions. We assumed $n = 10^k$, $k = 1, 2, 3, 4$ and $\alpha = 1.5$. The approximate values are computed by the formulas $\mathcal{R}^{(M)}_{\alpha,h}$ for $M = 1, 2, 3, 4$. We use uniform grid size $h = 0.1 \times 2^{-k}$, $k = 0, ..., 4$. For high dimensional cases the second-order formula fails whereas the 8th-order formula $\mathcal{R}^{(4)}_{\alpha,h}$ approximates with the predicted approximation rates.

In all the experiments we choose $\mathcal{D} = 5$ to have the saturation error comparable with the double precision rounding errors.

Table 3. Absolute errors and approximation rates for $\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})$ at $(1,1,0,\dots,0)$ using $\mathcal{R}_{\alpha,h}^{(M)}(\mathrm{e}^{-|\cdot|^2})$ with $\alpha = 1.5$, $n = 10^k$, $k = 1,2,3,4$ and $M = 1,2,3,4$.

	n	10		10^2		10^3		10^4	
	h^{-1}	error	rate	error	rate	error	rate	error	rate
$M=4$	10	0.964D-07		0.344D-06		0.645D-06		0.114D-05	
	20	0.434D-09	7.80	0.153D-08	7.81	0.287D-08	7.81	0.513D-08	7.80
	40	0.176D-11	7.95	0.619D-11	7.95	0.116D-10	7.95	0.207D-10	7.95
	80	0.696D-14	7.98	0.244D-13	7.99	0.457D-13	7.99	0.817D-13	7.99
	160	0.486D-16	8.00	0.118D-15	7.69	0.170D-15	8.07	0.313D-15	8.03
$M=3$	10	0.231D-05		0.827D-05		0.152D-04		0.234D-04	
	20	0.397D-07	5.86	0.142D-06	5.86	0.266D-06	5.84	0.474D-06	5.63
	40	0.636D-09	5.96	0.228D-08	5.96	0.426D-08	5.96	0.761D-08	5.96
	80	0.100D-10	5.99	0.358D-10	5.99	0.669D-10	5.99	0.120D-09	5.99
	160	0.157D-12	6.00	0.561D-12	6.00	0.105D-11	6.00	0.187D-11	6.00
$M=2$	10	0.701D-04		0.203D-03		0.262D-03		0.805D-04	
	20	0.461D-05	3.93	0.140D-04	3.86	0.251D-04	3.38	0.351D-04	1.20
	40	0.292D-06	3.98	0.889D-06	3.97	0.164D-05	3.94	0.288D-05	3.61
	80	0.183D-07	4.00	0.558D-07	3.99	0.103D-06	3.99	0.184D-06	3.97
	160	0.115D-08	4.00	0.349D-08	4.00	0.645D-08	4.00	0.115D-07	4.00
$M=1$	10	0.288D-02		0.239D-02					
	20	0.762D-03	1.92	0.118D-02	1.02				
	40	0.193D-03	1.98	0.365D-03	1.70	0.358D-03		0.805D-04	
	80	0.485D-04	1.99	0.964D-04	1.92	0.146D-03	1.29	0.789D-04	0.03
	160	0.121D-04	2.00	0.244D-04	1.98	0.421D-04	1.80	0.502D-04	0.65

Table 4. Absolute errors and approximation rates for $\mathcal{R}_\alpha(\mathrm{e}^{-|\cdot|^2})$ at $(0.8,0,0)$ using $\mathcal{R}_{\alpha,h}^{(3)}(\mathrm{e}^{-|\cdot|^2})$ with $\alpha = 1.5$ and $\alpha = 0.5$, for different h and $\mathcal{D}$.

		$\mathcal{D}=1$		$\mathcal{D}=2$		$\mathcal{D}=3$	
	h^{-1}	error	rate	error	rate	error	rate
$\alpha=1.5$	5	0.641D-04		0.102D-04		0.327D-04	
	10	0.205D-04	1.65	0.172D-06	5.90	0.585D-06	5.80
	20	0.702D-05	1.54	0.146D-08	6.87	0.949D-08	5.95
	40	0.246D-05	1.51	0.419D-09	1.81	0.150D-09	5.99
	80	0.869D-06	1.50	0.162D-09	1.37	0.233D-11	6.01
	160	0.307D-06	1.50	0.573D-10	1.50	0.311D-13	6.23
$\alpha=0.5$	5	0.202D-02		0.271D-04		0.871D-04	
	10	0.128D-02	0.65	0.212D-06	7.00	0.161D-05	5.75
	20	0.882D-03	0.54	0.163D-06	0.39	0.264D-07	5.93
	40	0.620D-03	0.51	0.116D-06	0.48	0.405D-09	6.03
	80	0.437D-03	0.50	0.816D-07	0.51	0.267D-11	7.25
	160	0.309D-03	0.50	0.576D-07	0.50	0.158D-11	0.63

In Table 4 we report on the absolute errors and the convergence rate of the 3-dimensional volume potential $\mathcal{R}_\alpha \mathrm{e}^{-|\cdot|^2}(0.8,0,0)$ with $\alpha = 1.5$ and $\alpha = 0.5$ using the cubature formulas $\mathcal{R}_{\alpha,h}^{(3)}$, for different values of h and $\mathcal{D}$. The results indicate approximations of order α if $\mathcal{D} = 1$ or $\mathcal{D} = 2$ and h is small, caused by the relatively large saturation error $\mathcal{O}(h^\alpha\, \mathrm{e}^{-\pi^2\mathcal{D}})$. If $\mathcal{D} = 3$ the rate of convergence 6 is obtained because the saturation error is negligible compared to the first term of the approximation error. On the other hand, due to the rapid decay of the functions η_{2M}, one has to take into account only a finite number of terms in the sum (4.1) to compute the value of $\mathcal{R}_\alpha f$ at a given point within a given accuracy, and the number of summands for fixed h increases in $\mathcal{D}$ ([20, p.65]).

For all the calculations the same quadrature rule is used for computing the one-dimensional integrals, the parameters are $a = 6$, $b = 5$, $\tau = 0.004$ and 600 summands in the quadrature sum.

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