On the computation of high-dimensional potentials of advection-diffusion operators

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Dedicated to Vladimir Maz'ya on the occasion of his 75th birthday

Abstract. We study a fast method for computing potentials of advection-diffusion operators $-\Delta + 2\mathbf{b} \cdot \nabla + c$ with $\mathbf{b} \in \mathbb{C}^n$ and $c \in \mathbb{C}$ over rectangular boxes in $\mathbb{R}^n$. By combining high-order cubature formulas with modern methods of structured tensor product approximations we derive an approximation of the potentials which is accurate and provides approximation formulas of high-order. The cubature formulas have been obtained by using the basis functions introduced in the theory of approximate approximations. The action of volume potentials on the basis functions allows one-dimensional integral representations with separable integrands, *i.e.* a product of functions depending only on 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 high-dimensional case.

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1 Introduction

The construction of efficient representations of multi-variate integral operators plays a crucial role in higher dimensional problems arising in a wide range of modern applications in physics, chemistry, financial mathematics, etc. Let us mention also multi-dimensional integral equations and volume potentials of elliptic and parabolic partial differential operators in $\mathbb{R}^n$, $n \geq 3$.

By combining high-order semi-analytic cubature formulas for volume potentials with modern methods of structured tensor product approximations we derive a method for approximating volume potentials which is accurate and fast also in very high dimensions and provides approximation formulas of high-order. The cubature formulas have been obtained by using the basis functions introduced in the theory of *approximate approximations* proposed by V. Maz'ya ([10], see also [11] and the reference therein). The development of *separated representations* (also called tensor structured representations) is due to Beylkin and Mohlenkamp ([2], [3]).

The action of volume potentials on the basis functions allows one-dimensional integral representations with separable integrands, *i.e.* a product of functions depending only on 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 high-dimensional case.

The construction of approximation formulas for the potential of the advection-diffusion operator $-\Delta+2\mathbf{b}\cdot\nabla+c$ with $\mathbf{b}\in\mathbb{C}^n$ and $c\in\mathbb{C}$ over the full space under the condition $\mathrm{Re}(c+|\mathbf{b}|^2)\geq 0$ was considered in [7]. Harmonic potentials over half-spaces were studied in [8]. Cubature formulas for advection-diffusion operators $-\Delta+c$ over boxes in $\mathbb{R}^n$, when $\mathrm{Re}\, c\geq 0$, were studied in [9]. In this paper we show how the method can be extended in order to treat the case $\mathrm{Re}(c+|\mathbf{b}|^2)<0$.

The outline is the following. In Section 2, after a brief introduction into cubature formulas based on approximate approximations and their error behavior, we describe the alghoritm for advection-diffusion potentials over the whole space. In Section 3, we derive the one dimensional integral representations of the advection-diffusion operator over boxes for our basis functions. In Section 4, for densities with separated representations, we describe a tensor product approximations of the integral operator. We provide results of numerical experiments showing that even for high space dimensions these approximations are accurate and preserve the predicted convergence order.

2 Advection-diffusion potentials over $\mathbb{R}^n$

We consider the volume potential of the advection-diffusion operator $-\Delta+2\mathbf{b}\cdot\nabla+c$ with $\mathbf{b}\in\mathbb{C}^n$ and $c\in\mathbb{C}$. We use the notation

$$\langle \mathbf{x},\mathbf{y}\rangle=\sum_{j=1}^{n} x_j y_j \qquad \text{and} \qquad |\mathbf{x}|^2=\langle \mathbf{x},\mathbf{x}\rangle.$$

If $\lambda^2=c+|\mathbf{b}|^2\neq 0$, then the fundamental solution can be given as

$$\kappa_\lambda(\mathbf{x})=\frac{\mathrm{e}^{\langle \mathbf{b},\mathbf{x}\rangle}}{(2\pi)^{n/2}}\left(\frac{|\mathbf{x}|}{\lambda}\right)^{1-n/2} K_{n/2-1}(\lambda|\mathbf{x}|),\ \lambda\in\mathbb{C}\setminus(-\infty,0],\ \mathbf{x}=(x_1,...,x_n)\neq 0$$

where K_ν is the modified Bessel function of the second kind ([1, 9.6]). If $\lambda^2=0$ then, for $n\geq 3$

$$\kappa_0(\mathbf{x})=\frac{\Gamma(n/2-1)}{4\pi^{n/2}}\frac{\mathrm{e}^{\langle \mathbf{b},\mathbf{x}\rangle}}{|\mathbf{x}|^{n-2}}.$$

A solution in $\mathbb{R}^n$ of the equation

$$(-\Delta+2\mathbf{b}\cdot\nabla+c)u=f$$

is given by the volume potential

$$u(\mathbf{x})=\mathcal{K}f(\mathbf{x})=\int_{\mathbb{R}^n}\kappa_\lambda(\mathbf{x}-\mathbf{y})f(\mathbf{y})\,d\mathbf{y}. \tag{2.1}$$

We construct an approximation of u if we replace the density f by functions with analytically known advection-diffusion potentials. Specifically we approximate the density $f \in C_0^N(\mathbb{R}^n)$ with the approximate quasi-interpolant

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

where h and $\mathcal{D}$ are positive parameters and η is a smooth and rapidly decaying function. The generating function η is chosen so that $\mathcal{K}_\lambda \eta$ can be computed, analytically or efficiently numerically. If the generating function η satisfies the moment condition of order N

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

then ([11, p.21])

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

with

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

Here $\mathcal{F}\eta$ denotes the Fourier transform of η

$$\mathcal{F}\eta(\mathbf{y}) = \int\limits_{\mathbb{R}^n} \eta(\mathbf{x}) \mathrm{e}^{-2i\pi \mathbf{x}\cdot\mathbf{y}} d\mathbf{x}.$$

Hence, for any *saturation error* $\varepsilon > 0$, one can fix the parameter $\mathcal{D}$ so that

$$|f(\mathbf{x}) - \mathcal{M}_{h,\mathcal{D}} f(\mathbf{x})| = \mathcal{O}((\sqrt{\mathcal{D}}h)^N + \varepsilon) ||f||_{W_\infty^N} \tag{2.4}$$

where W_∞^N denotes the Sobolev space of $L_\infty-$ functions whose generalized derivatives up to the order N also belong to L_∞. Then the linear combination

$$h^n \sum_{\mathbf{m}\in\mathbb{Z}^n} f(h\mathbf{m}) \int\limits_{\mathbb{R}^n} \kappa_\lambda (h\sqrt{\mathcal{D}} \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}} - \mathbf{y} \right)) \eta(\mathbf{y})\, d\mathbf{y}, \tag{2.5}$$

gives rise to a new class of semi-analytic cubature formulas with the property that, for any prescribed accuracy $\varepsilon > 0$, one can fix the parameter $\mathcal{D}$ so that (2.5) differs in some uniform or L_p-norm from the integral (2.1) by

$$\mathcal{O}((\sqrt{\mathcal{D}}h)^N + (\sqrt{\mathcal{D}}h)^2 \varepsilon) \qquad \text{as} \qquad h \to 0 \tag{2.6}$$

where N is determined by (2.3).

We assume the generating function as tensor product of one-dimensional functions

$$\eta_{2M}(\mathbf{x}) = \prod_{j=1}^n \widetilde{\eta}_{2M}(x_j); \qquad \widetilde{\eta}_{2M}(t) = \frac{(-1)^{M-1}}{2^{2M-1}\sqrt{\pi}(M-1)!} \frac{H_{2M-1}(t)\mathrm{e}^{-t^2}}{t} \tag{2.7}$$

where H_k are the Hermite polynomials

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

Under the condition $\mathrm{Re}(c + |\mathbf{b}|^2) \geq 0$, the following theorem gives an integral representation for the solution of

$$(-\Delta + 2\mathbf{b} \cdot \nabla + c)u = \prod_{j=1}^{n} \widetilde{\eta}_{2M}(x_j). \tag{2.8}$$

Theorem 2.1. *([7, p.896]) Let* $\mathrm{Re}(c + |\mathbf{b}|^2) \geq 0$, $n \geq 3$ *and* $M \geq 1$. *The solution of* (2.8) *can be expressed by the one-dimensional integral*

$$u(\mathbf{x}) = \frac{1}{4} \int_0^\infty \mathrm{e}^{-ct/4} \prod_{j=1}^{n} \frac{1}{\sqrt{\pi}} \mathrm{e}^{-(x_j - tb_j/2)^2/(1+t)} \mathcal{P}_M(t, x_j - \frac{t}{2} b_j) dt \tag{2.9}$$

where

$$\mathcal{P}_M(t, x) = \sum_{k=0}^{M-1} \frac{(-1)^k}{4^k k!} \frac{1}{(1+t)^{k+1/2}} H_{2k}\left(\frac{x}{\sqrt{1+t}}\right). \tag{2.10}$$

If $\mathrm{Re}(c + |\mathbf{b}|^2) > 0$ *then the representation* (2.9) *is valid for all* $n \geq 1$.

Remark 2.1. $\mathcal{P}_M(t, x)$ *are polynomials in* x *of degree* $2M - 2$. *For* $M = 1, 2, 3$, *they are given by*

$$\mathcal{P}_1(t,x) = \frac{1}{(1+t)^{1/2}}\,, \; \mathcal{P}_2(t,x) = \mathcal{P}_1(t,x) + \frac{1}{2(1+t)^{3/2}} - \frac{x^2}{(1+t)^{5/2}}\,,$$
$$\mathcal{P}_3(t,x) = \mathcal{P}_2(t,x) + \frac{3}{8(1+t)^{5/2}} - \frac{3\,x^2}{2(1+t)^{7/2}} + \frac{x^4}{2(1+t)^{9/2}}\,,$$
$$\mathcal{P}_4(t,x) = \mathcal{P}_3(t,x) - \frac{x^6}{6(t+1)^{13/2}} + \frac{5x^4}{4(t+1)^{11/2}} - \frac{15x^2}{8(t+1)^{9/2}} + \frac{5}{16(t+1)^{7/2}}.$$

The computation of the cubature formula (2.5) on the uniform grid $\{h\mathbf{k}\}$ leads to the discrete convolution

$$\mathcal{K}_h^{(M)} f(h\mathbf{k}) = \sum_{\mathbf{m} \in \mathbb{Z}^n} a_{\mathbf{k}-\mathbf{m}}^{(M)} f(h\mathbf{m}) \tag{2.11}$$

where we set

$$a_{\mathbf{k}}^{(M)} = \frac{1}{4(\pi\mathcal{D})^{n/2}} \int_0^\infty \mathrm{e}^{-ct/4} \prod_{j=1}^{n} \mathrm{e}^{-(k_j - tb_j/(2h))^2/(\mathcal{D}(1+t/(h^2\mathcal{D})))} \mathcal{P}_M\left(\frac{t}{h^2\mathcal{D}}, \frac{k_j}{\sqrt{\mathcal{D}}} - \frac{tb_j}{2h\sqrt{\mathcal{D}}}\right) dt. \tag{2.12}$$

For general functions f the most efficient summation methods for (2.11) are probably fast convolutions based on multi-variate FFT. However, even for the space dimension $n = 3$, problems of moderate size often exceed the capacity of computer systems. We propose a method which reduces the computational effort.

The computation of the sum (2.11) is very efficient for densities which allow a separated representation, *i.e.*, for given accuracy $\varepsilon > 0$, they can be represented as a sum of products of vectors in dimension 1

$$f(x_1, ..., x_n) = \sum_{p=1}^{R} r_p \prod_{j=1}^{n} f_j^{(p)}(x_j) + \mathcal{O}(\varepsilon). \tag{2.13}$$

Suppose that also the vectors $\{a_{\mathbf{k}}^{(M)}\}$ allow separated representations

$$a_{\mathbf{k}}^{(M)} = \sum_{q=1}^{Q} s_q \prod_{j=1}^{n} v_j^{(q)}(k_j) + \mathcal{O}(\varepsilon).$$

Then an approximate value of $\mathcal{K}f(h\mathbf{k})$ can be computed by the sum of products of one-dimensional convolutions

$$\mathcal{K}_h^{(M)} f(h\mathbf{k}) \approx \sum_{p=1}^{R} r_p \sum_{q=1}^{Q} s_q \prod_{j=1}^{n} \sum_{m_j \in \mathbb{Z}} v_j^{(q)}(k_j - m_j) f_j^{(p)}(hm_j).$$

Then the numerical computation of the integral does not require to perform an $n-$dimensional discrete convolution, for example, instead one has to compute nRQ one-dimensional discrete convolutions, which can lead to a considerable reduction of computing time and memory requirements, and gives the possibility to treat real world problems.

Following [6], a separated representation of the one-dimensional integrals $\{a_{\mathbf{k}}^{(M)}\}$ is obtained by applying an accurate quadrature rule. So the problem is reduced to finding efficient quadrature formulas for the parameter dependent integrals in (2.12). More precisely, one has to find a certain quadrature rule with minimal number of summands which approximates the integrals with prescribed error for the parameters $(k_j - m_j)/\sqrt{\mathcal{D}}$ within the range $|k_j - m_j| \leq K$ and some given bound K.

It is well known that the classical trapezoidal rule is exponentially converging for certain classes of integrands, for example periodic functions or rapidly decaying functions on the real line. As it was first observed in [13], if the integrand has the decay rate

$$|f(u)| \leq c \exp(-a \exp(|u|)) \qquad \text{for} \qquad |u| \to \infty$$

referred to as *doubly exponential decay*, then the trapezoidal rule is optimal with respect to the economy of the number of nodes.

We make the substitutions

$$t = \mathrm{e}^{\xi}, \quad \xi = \alpha(\sigma + \mathrm{e}^{\sigma}), \qquad \sigma = \beta(u - \mathrm{e}^{-u}) \tag{2.14}$$

with certain positive constants α, β, proposed by Waldvogel in [14]. Then the integrals in (2.12) are transformed to integrals over $\mathbb{R}$ with integrands decaying doubly exponentially in u.

After the substitution we have

$$a_{\mathbf{k}}^{(M)} = \frac{1}{4(\pi\mathcal{D})^{n/2}} \int_{-\infty}^{\infty} \mathrm{e}^{-c\Phi(u)/4} \Phi'(u)$$
$$\times \prod_{j=1}^{n} \mathrm{e}^{-(k_j - \Phi(u)b_j/(2h))^2/(\mathcal{D}(1+\Phi(u)/(h^2\mathcal{D})))} \mathcal{P}_M\left(\frac{\Phi(u)}{h^2\mathcal{D}}, \frac{k_j}{\sqrt{\mathcal{D}}} - \frac{\Phi(u)b_j}{2h\sqrt{\mathcal{D}}}\right) du$$

with

$$\begin{aligned}\Phi(u) &= \exp(\alpha\beta(u - \mathrm{e}^{-u}) + \alpha\exp(\beta(u - \mathrm{e}^{-u}))),\\ \Phi'(u) &= \Phi(u)\alpha\beta(1 + \mathrm{e}^{-u})(1 + \exp(\beta(u - \mathrm{e}^{-u}))).\end{aligned} \tag{2.15}$$

Application of the trapezoidal rule with step size τ and N_0, N_1 large positive integers gives

$$\begin{aligned}a_{\mathbf{k}}^{(M)} \approx & \frac{\tau}{4(\pi\mathcal{D})^{n/2}} \sum_{s=-N_0}^{N_1} \mathrm{e}^{-c\Phi(s\tau)/4}\Phi'(s\tau)\\ & \times \prod_{j=1}^{n} \mathrm{e}^{-(k_j - \Phi(s\tau)b_j/(2h))^2/(\mathcal{D}(1+\Phi(s\tau)/(h^2\mathcal{D})))} \mathcal{P}_M\left(\frac{\Phi(s\tau)}{h^2\mathcal{D}}, \frac{k_j}{\sqrt{\mathcal{D}}} - \frac{\Phi(s\tau)b_j}{2h\sqrt{\mathcal{D}}}\right).\end{aligned}$$

Assuming a separated representation (2.13) of the density we obtain the approximation of the n-dimensional convolutional sum in (2.11) via one-dimensional discrete convolutions

$$\begin{aligned}&\mathcal{K}_h^{(M)} f(h\mathbf{k}) \approx \frac{\tau}{4(\pi\mathcal{D})^{n/2}} \sum_{p=1}^{R} r_p \sum_{s=-N_0}^{N_1} \mathrm{e}^{-c\Phi(s\tau)/4}\Phi'(s\tau)\\ &\times \prod_{j=1}^{n} \sum_{m_j\in\mathbb{Z}} \mathrm{e}^{-(k_j - m_j - \Phi(s\tau)b_j/(2h))^2/(\mathcal{D}(1+\Phi(s\tau)/(h^2\mathcal{D})))} \mathcal{P}_M\left(\frac{\Phi(s\tau)}{h^2\mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{\Phi(s\tau)b_j}{2h\sqrt{\mathcal{D}}}\right) f_j^{(p)}(hm_j).\end{aligned}$$

3 One dimensional integral representations

We consider the integrals

$$\mathcal{K}_{[\mathbf{P},\mathbf{Q}]} f(\mathbf{x}) = \int\limits_{[\mathbf{P},\mathbf{Q}]} \kappa_\lambda(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d\mathbf{y} \tag{3.1}$$

taken over the hyper-rectangle

$$[\mathbf{P},\mathbf{Q}] = \{\mathbf{y} = (y_1, ..., y_n) \in \mathbb{R}^n : \; P_j \le y_j \le Q_j, \; j = 1, ..., n\} = \prod_{j=1}^{n} [P_j, Q_j].$$

Here we use the notations $\mathbf{P} = (P_1, ..., P_n)$ and $\mathbf{Q} = (Q_1, ..., Q_n)$.

The direct application of the method described in Section 2, which is based on replacing the density by a quasi-interpolant $\mathcal{M}_{h,\mathcal{D}} f$ and on the known values of $\mathcal{K}_{[\mathbf{P},\mathbf{Q}]}\eta$, does not give good approximations of (3.1). This is because the sum

$$\mathcal{M}_{h,\mathcal{D}} f(\mathbf{x}) = \mathcal{D}^{-n/2} \sum_{h\mathbf{m}\in[\mathbf{P},\mathbf{Q}]} f(h\mathbf{m}) \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right)$$

approximates f only in a subdomain of $[\mathbf{P},\mathbf{Q}]$ with positive distance from the boundary.

This difficulty can be overcome if we extend f with preserved smoothness outside $[\mathbf{P},\mathbf{Q}]$ and we approximate the extension $\widetilde{f}$ with the quasi-interpolant (2.2). Since η is smooth and of rapid decay, for any $\varepsilon > 0$ one can fix $r > 0$ and positive parameter $\mathcal{D} > 0$ so that the quasi-interpolant

$$\mathcal{M}_{h,\mathcal{D}}^{(r)} \widetilde{f}(\mathbf{x}) = \mathcal{D}^{-n/2} \sum_{h\mathbf{m}\in\Omega_{rh}} \widetilde{f}(h\mathbf{m}) \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right)$$

with $\Omega_{rh} = \prod_{j=1}^{n} I_j$, $I_j = (P_j - rh\sqrt{\mathcal{D}}, Q_j + rh\sqrt{\mathcal{D}})$, approximates f in $[\mathbf{P},\mathbf{Q}]$ with the error estimate (2.4).

We assume the tensor product basis functions (2.7). We deduce that the sum

$$h^n \sum_{h\mathbf{m}\in\Omega_{rh}} \widetilde{f}(h\mathbf{m}) \int\limits_{[\mathbf{P_m},\mathbf{Q_m}]} \kappa_\lambda\left(h\sqrt{\mathcal{D}}\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}-\mathbf{y}\right)\right)\prod_{j=1}^{n}\widetilde{\eta}_{2M}(y_j)\,d\mathbf{y}, \tag{3.2}$$

with $\mathbf{P_m} = (\mathbf{P}-h\mathbf{m})/(h\sqrt{\mathcal{D}})$ and $\mathbf{Q_m} = (\mathbf{Q}-h\mathbf{m})/(h\sqrt{\mathcal{D}})$, provides an approximation for $\mathcal{K}_{[\mathbf{P},\mathbf{Q}]}f(\mathbf{x})$ of high-order.

We are interested in integral representations of the solution of the advection-diffusion equation

$$(-\Delta + 2\mathbf{b}\cdot\nabla + c)\,u = \prod_{j=1}^{n}\chi_{(p_j,q_j)}(x_j)\,\widetilde{\eta}_{2M}(a_j x_j)\,. \tag{3.3}$$

Here $\chi_{(p_j,q_j)}$ is the characteristic function of the interval (p_j,q_j) with $-\infty \le p_j < q_j \le +\infty$, $j=1,\ldots,n$. As mentioned above, one-dimensional integral representations for the solution of (2.8) are known under the condition that $\mathrm{Re}\lambda^2 = \mathrm{Re}(c+|\mathbf{b}|^2) \ge 0$. The next Theorem allows to treat also the case $\mathrm{Re}\lambda^2 < 0$.

Theorem 3.1. *Let $\vartheta\in\mathbb{C}$, $\vartheta\neq 0$, be so that $\mathrm{Re}\,\vartheta \ge 0$ and $\mathrm{Re}(\lambda^2\vartheta)\ge 0$. If $n\ge 3$ the solution of the advection-diffusion equation (3.3) in $\mathbb{R}^n$ can be expressed by the one-dimensional integral*

$$u(\mathbf{x}) = \frac{\vartheta}{4}\int\limits_0^\infty \mathrm{e}^{-\vartheta ct/4}\prod_{j=1}^{n}(\Psi_M(a_j(x_j-\frac{b_j\vartheta t}{2}),a_j^2\vartheta t,a_j p_j)-\Psi_M(a_j(x_j-\frac{b_j\vartheta t}{2}),a_j^2\vartheta t,a_j q_j))dt \tag{3.4}$$

where

$$\Psi_M(x,t,y) = \frac{1}{2\sqrt{\pi}}\mathrm{e}^{-x^2/(1+t)}\left(\mathcal{P}_M(t,x)\,\mathrm{erfc}(F(t,x,y)) - \frac{\mathrm{e}^{-F^2(t,x,y)}}{\sqrt{\pi}}\mathcal{Q}_M(t,x,y)\right)$$

with $\mathcal{P}_M$ defined in (2.10),

$$\begin{aligned}
F(t,x,y) &= \sqrt{\frac{1+t}{t}}\Big(y-\frac{x}{1+t}\Big),\\
\mathcal{Q}_1(t,x,y) &= 0,\\
\mathcal{Q}_M(t,x,y) &= 2\sum_{k=1}^{M-1}\frac{(-1)^k}{k!\,4^k}\sum_{\ell=1}^{2k}\frac{(-1)^\ell}{t^{\ell/2}}\Bigg(H_{2k-\ell}(y)H_{\ell-1}\Big(\frac{y-x}{\sqrt{t}}\Big)\\
&\qquad -\binom{2k}{\ell}H_{2k-\ell}\Big(\frac{x}{\sqrt{1+t}}\Big)\frac{H_{\ell-1}\big(F(t,x,y)\big)}{(1+t)^{k+1/2}}\Bigg),\ M>1.
\end{aligned} \tag{3.5}$$

If $\mathrm{Re}(\lambda^2\vartheta) > 0$, then representation (3.4) is valid for all $n\ge 1$.

Proof. To treat the more general case $\mathrm{Re}\,\vartheta(c+|\mathbf{b}|^2)\ge 0$ we multiply (3.3) by ϑ and look for the solution of

$$(-\vartheta\Delta + 2\vartheta\mathbf{b}\cdot\nabla + \vartheta c)\,u = \vartheta\prod_{j=1}^{n}\chi_{(p_j,q_j)}(x_j)\,\widetilde{\eta}_{2M}(a_j x_j)\,. \tag{3.6}$$

If u satisfies (3.6) then $v = u\,\mathrm{e}^{-\langle \mathbf{b},\mathbf{x}\rangle}$ is solution of

$$(-\vartheta\Delta + \vartheta\lambda^2)\,v = \vartheta \mathrm{e}^{-\langle \mathbf{b},\mathbf{x}\rangle} \prod_{j=1}^{n} \chi_{(p_j,q_j)}(x_j)\,\widetilde{\eta}_{2M}(a_j x_j)\,. \tag{3.7}$$

We can obtain v by solving the Cauchy problem for the parabolic equation in $\mathbb{R}^n$

$$\partial_t w - \vartheta\Delta w + \vartheta\lambda^2 w = 0\,, \quad t > 0, \quad w(\mathbf{x},0) = \vartheta \mathrm{e}^{-\langle \mathbf{b},\mathbf{x}\rangle} \prod_{j=1}^{n} \chi_{(p_j,q_j)}(x_j)\,\widetilde{\eta}_{2M}(a_j x_j)\,. \tag{3.8}$$

Integrating in t we derive

$$w(\mathbf{x},T) - w(\mathbf{x},0) - \vartheta(\Delta - \lambda^2) \int_0^T w(\mathbf{x},t)\,dt = 0\,.$$

Hence the solution of (3.7) can be expressed as the one-dimensional integral

$$v(\mathbf{x}) = \int_0^\infty w(\mathbf{x},t)\,dt \tag{3.9}$$

provided the improper integral (3.9) exists. Obviously, if w solves (3.8), then $z = w\mathrm{e}^{\vartheta\lambda^2 t}$ is the solution of the initial value problem for the heat equation

$$\partial_t z - \vartheta\Delta z = 0\,, \quad z(\mathbf{x},0) = \vartheta \mathrm{e}^{-\langle \mathbf{b},\mathbf{x}\rangle} \prod_{j=1}^{n} \chi_{(p_j,q_j)}(x_j)\,\widetilde{\eta}_{2M}(a_j x_j)\,. \tag{3.10}$$

Because $\mathrm{Re}\,\vartheta \geq 0$, by Poisson's formula [5, p.209] the solution of (3.10) is for any $t > 0$

$$z(\mathbf{x},t) = \frac{\vartheta}{(4\pi\vartheta t)^{n/2}} \int_{[\mathbf{p},\mathbf{q}]} \mathrm{e}^{-|\mathbf{x}-\mathbf{y}|^2/(4\vartheta t)} \mathrm{e}^{-\langle \mathbf{b},\mathbf{y}\rangle} \prod_{j=1}^{n} \widetilde{\eta}_{2M}(a_j y_j)\,d\mathbf{y} \tag{3.11}$$

where $[\mathbf{p},\mathbf{q}]$ is the Cartesian product of the intervals $[p_j,q_j]$. Hence, if $\mathrm{Re}\,\lambda^2\vartheta > 0$, then the integral (3.9) with $w = z\mathrm{e}^{-\vartheta\lambda^2 t}$ exists for any $n \geq 1$, whereas for $\mathrm{Re}\,\lambda^2\vartheta = 0$ it exists due to the decay $t^{-n/2}$ only if $n \geq 3$. Using the relation [11, p.55]

$$\widetilde{\eta}_{2M}(a_j x_j) = \frac{1}{\sqrt{\pi}} \sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k a_j^{2k}} \frac{d^{2k}}{dx_j^{2k}} \mathrm{e}^{-(a_j x_j)^2}$$

we can express the integral (3.11), i.e. the solution of (3.10), as

$$z(\mathbf{x},t) = \frac{\vartheta \mathrm{e}^{\vartheta t|\mathbf{b}|^2 - \langle \mathbf{b},\mathbf{x}\rangle}}{(4\pi^2\vartheta t)^{n/2}} \prod_{j=1}^{n} \sum_{k=0}^{M-1} \frac{(-1)^k}{k!\,4^k a_j^{2k}} \int_{p_j}^{q_j} \mathrm{e}^{-(x_j - 2b_j\vartheta t - y_j)^2/(4\vartheta t)} \frac{d^{2k}}{dy_j^{2k}} \mathrm{e}^{-(a_j y_j)^2}\,dy_j\,.$$

Denoting by

$$I_k = \int\limits_{p_j}^{q_j} \mathrm{e}^{-(x_j-2b_j\vartheta t-y_j)^2/(4\vartheta t)} \, \frac{d^{2k}}{dy_j^{2k}} \mathrm{e}^{-(a_j y_j)^2} \, dy_j ,$$

integration by parts leads to

$$I_k = \frac{\partial^{2k}}{\partial x_j^{2k}} I_0 + \sum_{\ell=0}^{2k-1} (-1)^\ell \frac{\partial^\ell}{\partial y_j^\ell} \mathrm{e}^{-(x_j-2b_j\vartheta t-y_j)^2/(4\vartheta t)} \, \frac{\partial^{2k-\ell-1}}{\partial y_j^{2k-\ell-1}} \mathrm{e}^{-(a_j y_j)^2} \bigg|_{y_j=p_j}^{y_j=q_j} .$$

The definition of Hermite polynomials gives

$$\frac{\partial^{2k-\ell-1}}{\partial y_j^{2k-\ell-1}} \mathrm{e}^{-(a_j y_j)^2} = (-1)^{2k-\ell-1} a_j^{2k-\ell-1} \mathrm{e}^{-(a_j y_j)^2} H_{2k-\ell-1}(a_j y_j) ,$$

$$\frac{\partial^\ell}{\partial y_j^\ell} \mathrm{e}^{-(x_j-2b_j\vartheta t-y_j)^2/(4\vartheta t)} = \frac{(-1)^\ell \mathrm{e}^{-(x_j-2b_j\vartheta t-y_j)^2/(4\vartheta t)}}{(4\vartheta t)^{\ell/2}} \, H_\ell\Big(\frac{y_j - x_j + 2b_j\vartheta t}{(4\vartheta t)^{1/2}} \Big).$$

Therefore

$$I_k = \frac{\partial^{2k}}{\partial x_j^{2k}} I_0 + a_j^{2k} \sum_{\ell=0}^{2k-1} \frac{(-1)^{\ell+1}}{(4\vartheta t)^{\ell/2} a_j^{\ell+1}} \widetilde{H}_\ell\Big(\frac{y_j - x_j + 2b_j\vartheta t}{(4\vartheta t)^{1/2}} \Big) \widetilde{H}_{2k-\ell-1}(a_j y_j) \bigg|_{y_j=p_j}^{y_j=q_j} ,$$

where we use the abbreviation

$$\widetilde{H}_\ell(y) = \mathrm{e}^{-y^2} H_\ell(y) . \tag{3.12}$$

We have

$$I_0 = \frac{\mathrm{e}^{-a_j^2(x_j-2b_j\vartheta t)^2/(1+4a_j^2\vartheta t)}}{2} \sqrt{\frac{4\pi\vartheta t}{1+4a_j^2\vartheta t}} \big(\operatorname{erfc}(f_j(p_j)) - \operatorname{erfc}(f_j(q_j)) \big) ,$$

where we denote

$$f_j(y) = F(4a_j^2\vartheta t, a_j(x_j - 2b_j\vartheta t), a_j y). \tag{3.13}$$

In view of

$$\frac{d^\ell}{dz^\ell} \operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} (-1)^\ell \mathrm{e}^{-z^2} H_{\ell-1}(z) = \frac{2}{\sqrt{\pi}} (-1)^\ell \widetilde{H}_{\ell-1}(z), \quad \ell \geq 1 ,$$

one gets for $\ell < 2k$

$$\frac{\partial^{2k-\ell}}{\partial x_j^{2k-\ell}} \operatorname{erfc}(f_j(y)) = \frac{(-1)^{2k-\ell}}{(4\vartheta t(1+4a_j^2\vartheta t))^{k-\ell/2}} \left[\frac{d^{2k-\ell}}{dz^{2k-\ell}} \operatorname{erfc}(z) \right]_{z=f_j(y)} = \frac{2\widetilde{H}_{2k-\ell-1}(f_j(y))}{\sqrt{\pi}(4\vartheta t(1+4a_j^2\vartheta t))^{k-\ell/2}} .$$

Therefore, since

$$\frac{\partial^\ell}{\partial x_j^\ell} \mathrm{e}^{-a_j^2(x_j-2b_j\vartheta t)^2/(1+4a_j^2\vartheta t)} = \frac{(-1)^\ell a_j^\ell}{(1+4a_j^2\vartheta t)^{\ell/2}} \widetilde{H}_\ell\Big(\frac{a_j(x_j - 2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}} \Big) ,$$

we obtain

$$\frac{1}{\sqrt{\pi\vartheta t}}\frac{\partial^{2k}}{\partial x_j^{2k}}I_0 = \frac{a_j^{2k}}{(1+4a_j^2\vartheta t)^{k+1/2}}\widetilde{H}_{2k}\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big)\operatorname{erfc}(f_j(y))\Big|_{y=q_j}^{y=p_j}$$
$$-\frac{2}{\sqrt{\pi}(1+4a_j^2\vartheta t)^{k+1/2}}\sum_{\ell=0}^{2k-1}\binom{2k}{\ell}\frac{(-1)^\ell a_j^\ell}{(4\vartheta t)^{k-\ell/2}}\widetilde{H}_\ell\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big)\widetilde{H}_{2k-\ell-1}(f_j(y))\Big|_{y=p_j}^{y=q_j}.$$

Hence, $z(\mathbf{x},t)$ can be written in the form

$$z(\mathbf{x},t) = \frac{\vartheta e^{\vartheta t|\mathbf{b}|^2-\langle\mathbf{b},\mathbf{x}\rangle}}{\pi^{n/2}}\prod_{j=1}^n\Bigg(\frac{1}{2}\operatorname{erfc}(f_j(y))\Big|_{y=q_j}^{y=p_j}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!\,4^k(1+4a_j^2\vartheta t)^{k+1/2}}\widetilde{H}_{2k}\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big)$$
$$+\frac{1}{\sqrt{\pi}}\sum_{k=1}^{M-1}\frac{(-1)^k}{k!\,4^k}\sum_{\ell=0}^{2k-1}\frac{(-1)^\ell}{(4a_j^2\vartheta t)^{k-\ell/2}}\Bigg(\widetilde{H}_\ell(a_jy)\widetilde{H}_{2k-\ell-1}\Big(\frac{y-x_j+2b_j\vartheta t}{\sqrt{4\vartheta t}}\Big)$$
$$-\binom{2k}{\ell}\widetilde{H}_\ell\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big)\frac{\widetilde{H}_{2k-\ell-1}(f_j(y))}{(1+4a_j^2\vartheta t)^{k+1/2}}\Bigg)\Bigg|_{y=p_j}^{y=q_j}\Bigg).$$

From (3.12) we have

$$\widetilde{H}_{2k}\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big) = e^{-(a_j^2(x_j-2b_j\vartheta t)^2)/(1+4a_j^2\vartheta t)}H_{2k}\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big);$$
$$\widetilde{H}_\ell(a_jy)\widetilde{H}_{2k-\ell-1}\Big(\frac{y-x_j+2b_j\vartheta t}{\sqrt{4\vartheta t}}\Big)$$
$$= e^{-f_j^2(y)}e^{-(a_j^2(x_j-2b_j\vartheta t)^2)/(1+4a_j^2\vartheta t)}H_\ell(a_jy)H_{2k-\ell-1}\Big(\frac{y-x_j+2b_j\vartheta t}{\sqrt{4\vartheta t}}\Big).$$

Thus we obtain

$$u(\mathbf{x}) = \int_0^\infty e^{-\vartheta\lambda^2 t}e^{\langle\mathbf{b},\mathbf{x}\rangle}z(\mathbf{x},t)\,dt = \int_0^\infty \vartheta e^{-\vartheta\lambda^2 t}e^{\vartheta t|\mathbf{b}|^2}\prod_{j=1}^n\frac{e^{-(a_j^2(x_j-2b_j\vartheta t)^2)/(1+4a_j^2\vartheta t)}}{\sqrt{\pi}}$$
$$\times\Bigg(\frac{1}{2}\operatorname{erfc}(f_j(y))\Big|_{y=q_j}^{y=p_j}\sum_{k=0}^{M-1}\frac{(-1)^k}{k!\,4^k(1+4a_j^2\vartheta t)^{k+1/2}}H_{2k}\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big)$$
$$+\frac{e^{-f_j^2(y)}}{\sqrt{\pi}}\sum_{k=1}^{M-1}\frac{(-1)^k}{k!\,4^k}\sum_{\ell=1}^{2k}\frac{(-1)^\ell}{(4a_j^2\vartheta t)^{\ell/2}}\Bigg(H_{2k-\ell}(a_jy)H_{\ell-1}\Big(\frac{y-x_j+2b_j\vartheta t}{(4\vartheta t)^{1/2}}\Big)$$
$$-\binom{2k}{\ell}H_{2k-\ell}\Big(\frac{a_j(x_j-2b_j\vartheta t)}{(1+4a_j^2\vartheta t)^{1/2}}\Big)\frac{H_{\ell-1}(f_j(y))}{(1+4a_j^2\vartheta t)^{k+1/2}}\Bigg)\Bigg|_{y=p_j}^{y=q_j}\Bigg)dt.$$

Therefore, keeping in mind (3.13), (2.10) and (3.5), we find

$$u(\mathbf{x}) = \int_0^\infty \vartheta e^{-\vartheta ct}\prod_{j=1}^n\frac{e^{-a_j^2(x_j-2b_j\vartheta t)^2/(1+4a_j^2\vartheta t)}}{2\sqrt{\pi}}\times$$
$$\Bigg(\mathcal{P}_M(4a_j^2\vartheta t, a_j(x_j-2b_j\vartheta t))\operatorname{erfc}(f_j(y)) - \frac{e^{-f_j^2(y)}}{\sqrt{\pi}}\mathcal{Q}_M(4a_j^2\vartheta t, a_j(x_j-2b_j\vartheta t), a_jy)\Bigg)\Bigg|_{y=q_j}^{y=p_j}dt$$

and the assertion follows. $\square$

Remark 3.1. *If $M>1$, $\mathcal{Q}_M$ are polynomials in x of degree $2M-3$. For example, for $M=2,3$*

$$\mathcal{Q}_2(t,x,p)=\frac{\sqrt{t}}{(1+t)}\Big(\frac{x}{1+t}+p\Big),$$
$$\mathcal{Q}_3(t,x,p)=-\frac{\sqrt{t}}{4(1+t)}\Big(\frac{2x^3}{(1+t)^3}+\frac{2px^2-5x}{(1+t)^2}+\frac{(2p^2-5)x-3p}{1+t}+p(2p^2-7)\Big).$$

4 Tensor product cubature formulas and numerical results

We compute the cubature formula (3.2) using the integral representation of Theorem 3.1. At the grid points $\{h\mathbf{k}\}$ we obtain

$$\mathcal{K}_{[\mathbf{P},\mathbf{Q}]}f(h\mathbf{k})\approx\sum_{h\mathbf{m}\in\Omega_{rh}}c^{(M)}_{\mathbf{k},\mathbf{m}}\widetilde{f}(h\mathbf{m}) \tag{4.1}$$

where we set

$$\begin{aligned}c^{(M)}_{\mathbf{k},\mathbf{m}}&=h^n\int\limits_{[\mathbf{P_m},\mathbf{Q_m}]}\kappa_\lambda\left(h\sqrt{\mathcal{D}}\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}-\mathbf{y}\right)\right)\prod_{j=1}^n\widetilde{\eta}_{2M}(y_j)\,d\mathbf{y}\\ &=\frac{\vartheta}{4\mathcal{D}^{n/2}}\int\limits_0^\infty\mathrm{e}^{-\vartheta ct/4}\prod_{j=1}^n\Bigg((\Psi_M\left(\frac{k_j-m_j}{\sqrt{\mathcal{D}}}-\frac{b_j\vartheta t}{2h\sqrt{\mathcal{D}}},\frac{\vartheta t}{h^2\mathcal{D}},\frac{P_j-hm_j}{h\sqrt{\mathcal{D}}}\right)\\ &\qquad-\Psi_M\left(\frac{k_j-m_j}{\sqrt{\mathcal{D}}}-\frac{b_j\vartheta t}{2h\sqrt{\mathcal{D}}},\frac{\vartheta t}{h^2\mathcal{D}},\frac{Q_j-hm_j}{h\sqrt{\mathcal{D}}}\right)\Bigg)\,dt.\end{aligned}$$

We can speed up the computation of (4.1) if we use the approximation ([9, p.175])

$$\Psi_M(x,t,p)-\Psi_M(x,t,q)\approx\begin{cases}0\,, & p,q\geq r \text{ or } p,q\leq -r\,,\\ \mathrm{e}^{-x^2/(1+t)}\mathcal{P}_M(t,x), & p\leq -r \text{ and } q\geq r\,,\end{cases}$$

with the error $\mathcal{O}(\mathrm{e}^{-r^2})$. Similarly, if $q-p\geq 2r$, then

$$\Psi_M(x,t,p)-\Psi_M(x,t,q)\approx\begin{cases}\Psi_M(x,t,p)\,, & -r<p<r\,,\\ \mathrm{e}^{-x^2/(1+t)}\mathcal{P}_M(t,x)-\Psi_M(x,t,q), & -r<q<r\,.\end{cases}$$

Therefore, for appropriately chosen $r>0$ we can set, within a given accuracy, if $p-hm\leq -rh\sqrt{\mathcal{D}}$,

$$\Psi_M\left(\frac{k}{\sqrt{\mathcal{D}}}-\frac{b\vartheta t}{2h\sqrt{\mathcal{D}}},\frac{t\vartheta}{h^2\mathcal{D}},\frac{p-hm}{h\sqrt{\mathcal{D}}}\right)=\mathrm{e}^{-(k-b\vartheta t/(2h))^2/(\mathcal{D}(1+t/(h^2\mathcal{D}))}\mathcal{P}_M\left(\frac{t\vartheta}{h^2\mathcal{D}},\frac{k}{\sqrt{\mathcal{D}}}-\frac{b\vartheta t}{2h\sqrt{\mathcal{D}}}\right),$$

whereas, for $q-hm\geq rh\sqrt{\mathcal{D}}$,

$$\Psi_M\left(\frac{k}{\sqrt{\mathcal{D}}}-\frac{b\vartheta t}{2h\sqrt{\mathcal{D}}},\frac{t\vartheta}{h^2\mathcal{D}},\frac{q-hm}{h\sqrt{\mathcal{D}}}\right)=0.$$

We deduce that we can split the sum (4.1) into

$$\mathcal{K}_{[\mathbf{P},\mathbf{Q}]}f(h\mathbf{k}) \approx \sum_{h\mathbf{m}\in\widetilde{\Omega}_{rh}} b^{(M)}_{\mathbf{k}-\mathbf{m}} f(h\mathbf{m}) + \sum_{h\mathbf{m}\in\Omega_{rh}\setminus\widetilde{\Omega}_{rh}} c^{(M)}_{\mathbf{k},\mathbf{m}} \widetilde{f}(h\mathbf{m}) \tag{4.2}$$

where $\widetilde{\Omega}_{rh} = \prod_{j=1}^{n} \widetilde{I}_j$, $\widetilde{I}_j = (P_j + rh\sqrt{\mathcal{D}}, Q_j - rh\sqrt{\mathcal{D}})$ and

$$b^{(M)}_{\mathbf{k}} = \frac{\vartheta}{4(\pi\mathcal{D})^{n/2}} \int_0^\infty \mathrm{e}^{-\vartheta ct/4} \mathrm{e}^{-(k_j - t\vartheta b_j/(2h))^2/(\mathcal{D}(1+t\vartheta/(h^2\mathcal{D})))} \mathcal{P}_M\left(\frac{t\vartheta}{h^2\mathcal{D}}, \frac{k_j}{\sqrt{\mathcal{D}}} - \frac{t\vartheta b_j}{2h\sqrt{\mathcal{D}}}\right) dt.$$

The one-dimensional integrals of $b^{(M)}_{\mathbf{k}-\mathbf{m}}$ and $c^{(M)}_{\mathbf{k},\mathbf{m}}$ are transformed to integrals over the real line with integrands decaying doubly exponentially by making the substitution (2.15). The quadrature rule with step τ gives

$$b^{(M)}_{\mathbf{k}} \approx \frac{\tau\vartheta}{4(\pi\mathcal{D})^{n/2}} \times$$
$$\sum_{s=-N_0}^{N_1} \mathrm{e}^{-\vartheta c\Phi(s\tau)/4} \Phi'(s\tau) \mathrm{e}^{-(k_j - \Phi(s\tau)\vartheta b_j/(2h))^2/(\mathcal{D}(1+\Phi(s\tau)\vartheta/(h^2\mathcal{D})))} \mathcal{P}_M\left(\frac{\Phi(s\tau)\vartheta}{h^2\mathcal{D}}, \frac{k_j}{\sqrt{\mathcal{D}}} - \frac{\Phi(s\tau)\vartheta b_j}{2h\sqrt{\mathcal{D}}}\right);$$

$$c^{(M)}_{\mathbf{k},\mathbf{m}} \approx \frac{\tau\vartheta}{4\mathcal{D}^{n/2}} \sum_{s=-N_0}^{N_1} \mathrm{e}^{-\vartheta c\Phi(s\tau)/4} \Phi'(s\tau) \prod_{j=1}^{n} \left(\Psi_M\left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{b_j\vartheta\Phi(s\tau)}{2h\sqrt{\mathcal{D}}}, \frac{\vartheta\Phi(s\tau)}{h^2\mathcal{D}}, \frac{P_j - hm_j}{h\sqrt{\mathcal{D}}}\right)\right.$$
$$\left. - \Psi_M\left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{b_j\vartheta\Phi(s\tau)}{2h\sqrt{\mathcal{D}}}, \frac{\vartheta\Phi(s\tau)}{h^2\mathcal{D}}, \frac{Q_j - hm_j}{h\sqrt{\mathcal{D}}}\right)\right).$$

Let us assume a separated representation (2.13) of the density $f \in C^N([\mathbf{P},\mathbf{Q}])$. An extension of $f^{(p)}_j(x_j)$ outside the interval $[P_j, Q_j]$, with preserved smoothness, can be obtained by using the following formula proposed by Hestenes ([4], see also [12, p.19])

$$\widetilde{f}^{(p)}_j(x_j) = \begin{cases} \sum\limits_{s=1}^{N} c_s f^{(p)}_j(-a_s(x_j - Q_j) + Q_j), & Q_j < x_j \le Q_j + \dfrac{Q_j - P_j}{A} \\ f^{(p)}_j(x_j), & P_j \le x_j \le Q_j \\ \sum\limits_{s=1}^{N} c_s f^{(p)}_j(-a_s(x_j - P_j) + P_j), & P_j - \dfrac{Q_j - P_j}{A} \le x_j < P_j \end{cases}$$

with $\{a_s\}, s = 1, ..., N+1$, different positive constants, $A = \max_{1\le s\le N+1} a_s$ and the coefficients $\{c_s\}$ are solutions of the system

$$\sum_{s=1}^{N+1} c_s(-a_s)^k = 1, \qquad k = 0, ..., N.$$

The extension $\widetilde{f}$ preserves smoothness and

$$||\widetilde{f}||_{W^N_\infty(\Omega_{rh})} \le C||f||_{W^N_\infty([\mathbf{P},\mathbf{Q}])}, \qquad C > 0.$$

Then the linear combination (4.2) approximates (3.1) with the asymptotic error (2.6).

We derive the approximation of the convolutional sum in (4.2) via one-dimensional discrete convolutions

$$\sum_{h\mathbf{m}\in\widetilde{\Omega}_{rh}} b^{(M)}_{\mathbf{k}-\mathbf{m}} f(h\mathbf{m}) \approx \frac{\tau\vartheta}{4(\pi\mathcal{D})^{n/2}} \sum_{p=1}^{R} r_p \sum_{s=-N_0}^{N_1} \mathrm{e}^{-\vartheta c\Phi(s\tau)/4}\Phi'(s\tau) \prod_{j=1}^{n} \sum_{hm_j\in\widetilde{I}_j} f_j^{(p)}(hm_j)\times$$
$$\mathrm{e}^{-(k_j-m_j-\Phi(s\tau)\vartheta b_j/(2h))^2/(\mathcal{D}(1+\Phi(s\tau)\vartheta/(h^2\mathcal{D})))}\mathcal{P}_M\left(\frac{\Phi(s\tau)\vartheta}{h^2\mathcal{D}}, \frac{k_j-m_j}{\sqrt{\mathcal{D}}} - \frac{b_j\vartheta\Phi(s\tau)}{2h\sqrt{\mathcal{D}}}\right)$$

and the approximation of the second sum in (4.2) using one dimensional operations

$$\sum_{h\mathbf{m}\in\Omega_{rh}\setminus\widetilde{\Omega}_{rh}} c^{(M)}_{\mathbf{k},\mathbf{m}} \widetilde{f}(h\mathbf{m}) \approx \frac{\tau\vartheta}{4\mathcal{D}^{n/2}} \sum_{p=1}^{R} r_p \sum_{s=-N_0}^{N_1} \mathrm{e}^{-\vartheta c\Phi(s\tau)/4}\Phi'(s\tau)$$
$$\times \prod_{j=1}^{n} \sum_{hm_j\in I_j\setminus\widetilde{I}_j} \widetilde{f}_j^{(p)}(hm_j)\Psi_M\left(\frac{k_j-m_j}{\sqrt{\mathcal{D}}} - \frac{b_j\vartheta\Phi(s\tau)}{2h\sqrt{\mathcal{D}}}, \frac{\vartheta\Phi(s\tau)}{h^2\mathcal{D}}, \frac{X}{h\sqrt{\mathcal{D}}}\right)\Bigg|_{X=Q_j-hm_j}^{X=P_j-hm_j}.$$

We have tested the approximation of the potential (2.1) with $\mathbf{b} = 0$, the exact solution $u(\mathbf{x}) = \prod_{j=1}^{n} v(x_j)$ and the density

$$\begin{aligned} f(\mathbf{x}) &= (-\Delta + c)\prod_{j=1}^{n} v(x_j) = \sum_{p=1}^{n}\prod_{j=1}^{n} f_j^{(p)}(x_j), \qquad \mathbf{x}\in[-1,1]^n\,, \\ &\text{where}\quad f_j^{(p)}(x) = v(x) \quad \text{if} \quad j\neq p\,, \quad f_j^{(p)}(x) = -v''(x) + \frac{c}{n}v(x) \quad \text{if} \quad j = p. \end{aligned} \tag{4.3}$$

We assumed $\mathcal{D} = 4$ in order to have the saturation error comparable with the double precision rounding errors. We choose the parameters $\alpha = 2$, $\beta = 2$ in (2.14) and $\tau = 0.005$, $N_0 = 200$, $N_1 = 300$ in the trapezoidal rule.

In Table 1 we compare exact and approximate values for $\mathcal{K}f$ at some points $(x_1, 0, ..., 0)$ for space dimensions $n = 3, 30, 300, 3000, 30000$, with $v(x) = \mathrm{e}^x(1-x^2)^2$, $c = \mathrm{e}^{2i\pi/3}$ and $\vartheta = \mathrm{e}^{-i\pi/3}$. We choose $M = 3$ and $h = 0.0125$, We provide results for the Hestenes extension corresponding to $a_s = 1/s$. The numerical results coincide with those if using $\widetilde{f}_j^{(p)} = f_j^{(p)}$ or other two Hestenes extensions with $a_s = 1/2^s$ or $a_s = s$. The computational time on a 2 cpu Xeon Quad-Core processor with 2.4 Ghz is 3.6 seconds for any space dimension n. It does not depend on n because of the special choice (4.3), which requires the computation of $2(N_0 + N_1)$ one-dimensional convolutions and summations. For general f in (2.13), the approximation of the potential requires to compute $nR(N_0 + N_1)$ of those one-dimensional operations. Thus the computational time scales linearly in the space dimension n.

In Tables 2 and 3 we report on the absolute error and the approximation rates for (2.1) when $c = -1 + 4i$, in dimension $n = 3, 10, 10^2, 10^4, 10^5$. We used the approximation formulas of order 2, 4, 6. We provide results when f is given in (4.3) with $v(x) = \cos^2(\pi x/2)$ and $\widetilde{f}_j^{(p)} = f_j^{(p)}$ (Table 2), and with $v(x) = \mathrm{e}^x(1-x^2)^2$ and the Hestenes extension corresponding to $a_s = 1/2^s$ (Table 3). For very high dimensional case the second order formula fails but the $6-th$ order formula approximates with the predicted approximation rate.

dimension	x_1	exact value	approximation	absolute error
$n = 3$	0.0	1.0000000000000000	0.99999999994469568	0.566E-09
	0.2	1.1256447819204123	1.1256447819202458	0.586E-09
	0.4	1.0526315066556802	1.0526315066750866	0.597E-09
	0.6	0.74633986063995228	0.74633986062252122	0.592E-09
	0.8	0.28843010433262362	0.28843010422945359	0.576E-09
$n = 30$	0.0	1.0000000000000000	1.0000000057417306	0.574E-08
	0.2	1.1256447819204123	1.1256447884781275	0.656E-08
	0.4	1.0526315066556802	1.0526315129819730	0.633E-08
	0.6	0.74633986063995228	0.74633986550526243	0.487E-08
	0.8	0.28843010433262362	0.28843010690023407	0.257E-08
$n = 300$	0.0	1.0000000000000000	1.0000000574634069	0.575E-07
	0.2	1.1256447819204123	1.1256448466982212	0.648E-07
	0.4	1.0526315066556802	1.0526315674272828	0.608E-07
	0.6	0.74633986063995228	0.74633990412891404	0.435E-07
	0.8	0.28843010433262362	0.28843012197182266	0.176E-07
$n = 3000$	0.0	1.0000000000000000	1.0000005744371889	0.574E-06
	0.2	1.1256447819204123	1.1256454286274939	0.647E-06
	0.4	1.0526315066556802	1.0526321116120156	0.605E-06
	0.6	0.74633986063995228	0.74634028996878954	0.429E-06
	0.8	0.28843010433262362	0.28843027108409619	0.167E-06
$n = 30000$	0.0	1.0000000000000000	1.0000057444699280	0.574E-05
	0.2	1.1256447819204123	1.1256512482478720	0.647E-05
	0.4	1.0526315066556802	1.0526375537513712	0.605E-05
	0.6	0.74633986063995228	0.74634414857030773	0.429E-05
	0.8	0.28843010433262362	0.28843176227718131	0.166E-05

Table 1: Exact and approximated values of $\mathcal{K}f(x_1, 0, ..., 0)$ and the absolute error using (4.2) with $M = 3$ and $h = 0.0125$. The density f is given in (4.3) with $v(x) = \mathrm{e}^x(1 - x^2)^2$.

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$M = 1$

n	3		10		10^2		10^4		10^5	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.539E-01		0.177E+00		0.496E+00		0.500E+00		0.500E+00	
20	0.143E-01	1.92	0.527E-01	1.75	0.351E+00	0.49	0.500E+00	0.00	0.500E+00	0.00
40	0.363E-02	1.98	0.138E-01	1.93	0.131E+00	1.42	0.500E+00	0.00	0.500E+00	0.00
80	0.910E-03	1.99	0.349E-02	1.98	0.367E-01	1.84	0.500E+00	0.00	0.500E+00	0.00
160	0.228E-03	1.99	0.875E-03	1.99	0.945E-02	1.96	0.427E+00	0.23	0.500E+00	0.00

$M = 2$

n	3		10		10^2		10^4		10^5	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.269E-02		0.103E-01		0.101E+00		0.500E+00		0.500E+00	
20	0.177E-03	3.93	0.680E-03	3.92	0.736E-02	3.78	0.388E+00	0.36	0.500E+00	0.00
40	0.112E-04	3.98	0.430E-04	3.98	0.469E-03	3.97	0.452E-01	3.10	0.306E+00	0.71
80	0.702E-06	3.99	0.270E-05	3.99	0.294E-04	3.99	0.296E-02	3.93	0.288E-01	3.41
160	0.439E-07	3.99	0.169E-06	3.99	0.184E-05	3.99	0.186E-03	3.99	0.185E-02	3.96

$M = 3$

n	3		10		10^2		10^4		10^5	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.879E-04		0.338E-03		0.367E-02		0.262E+00		0.500E+00	
20	0.145E-05	5.92	0.558E-05	5.92	0.608E-04	5.92	0.611E-02	5.42	0.578E-01	3.11
40	0.230E-07	5.98	0.884E-07	5.98	0.964E-06	5.98	0.973E-04	5.97	0.973E-03	5.89
80	0.361E-09	5.99	0.139E-08	5.99	0.151E-07	5.99	0.153E-05	5.99	0.153E-04	5.99
160	0.565E-11	5.99	0.217E-10	5.99	0.236E-09	5.99	0.239E-07	5.99	0.238E-06	5.99

Table 2: Absolute errors and approximation rates for $\mathcal{K}f(0.5, 0, ..., 0)$ using (4.2) and the density f given in (4.3) with $v(x) = \cos^2(\pi x/2)$, $\widetilde{f}_j^{(p)}(x) = f_j^{(p)}(x)$, $c = -1 + 4i$.

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$M = 1$

n	3		10		10^2		10^4		10^5	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.288E+00		0.375E+00		0.112E+01		0.118E+01		0.118E+01	
20	0.737E-01	1.97	0.106E+00	1.82	0.629E+00	0.84	0.118E+01	0.00	0.118E+01	0.00
40	0.185E-01	1.99	0.274E-01	1.95	0.204E+00	1.62	0.118E+01	0.00	0.118E+01	0.00
80	0.464E-02	1.99	0.689E-02	1.99	0.548E-01	1.90	0.117E+01	0.01	0.118E+01	0.00
160	0.116E-02	1.99	0.173E-02	1.99	0.139E-01	1.97	0.812E+00	0.52	0.118E+01	0.00

$M = 2$

n	3		10		10^2		10^4		10^5	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.107E-01		0.564E-02		0.239E-01		0.921E+00		0.118E+01	
20	0.668E-03	4.00	0.295E-03	4.26	0.926E-03	4.68	0.544E-01	4.08	0.442E+00	1.41
40	0.416E-04	4.00	0.175E-04	4.07	0.490E-04	4.24	0.261E-02	4.38	0.256E-01	4.10
80	0.260E-05	4.00	0.108E-05	4.02	0.293E-05	4.06	0.150E-03	4.12	0.148E-02	4.11
160	0.162E-06	4.00	0.674E-07	4.00	0.181E-06	4.02	0.914E-05	4.03	0.906E-04	4.03

$M = 3$

n	3		10		10^2		10^4		10^5	
h^{-1}	error	rate	error	rate	error	rate	error	rate	error	rate
10	0.272E-03		0.708E-03		0.629E-02		0.806E+00			
20	0.420E-05	6.01	0.108E-04	6.03	0.952E-04	6.04	0.935E-02	6.43	0.969E-01	
40	0.654E-07	6.00	0.168E-06	6.00	0.148E-05	6.01	0.145E-03	6.02	0.145E-02	6.06
80	0.105E-08	5.97	0.261E-08	6.00	0.230E-07	6.00	0.225E-05	6.00	0.225E-04	6.00
160	0.142E-10	6.20	0.413E-10	5.98	0.360E-09	6.00	0.352E-07	6.00	0.352E-06	5.99

Table 3: Absolute errors and approximation rates for $\mathcal{K}f(0.3, 0.4, 0, ..., 0)$ using (4.2) and f given in (4.3) with $v(x) = \mathrm{e}^x(1 - x^2)^2$ and the Hestenes extension corresponding to $a_s = 1/2^s$, $c = -1 + 4i$.