

Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint

ISSN 2198-5855

**Approximation of solutions to multidimensional parabolic
equations by approximate approximations**

Flavia Lanzara¹, Vladimir Maz'ya², Gunther Schmidt³

submitted: June 10, 2015

¹ Department of Mathematics
Sapienza University of Rome
Piazzale Aldo Moro 2
00185 Rome
Italy
E-Mail: lanzara@mat.uniroma1.it

² Department of Mathematics
University of Linköping
581 83 Linköping
Sweden
E-Mail: vlmaz@mai.liu.se *and*
Department of Mathematical Sciences
M&O Building
University of Liverpool
UK

³ Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: gunther.schmidt@wias-berlin.de

No. 2119
Berlin 2015



2010 *Mathematics Subject Classification.* 65D32, 41A63, 41A30, 65-05.

Key words and phrases. Higher dimensions, parabolic equation, heat potential, separated representations, tensor product approximation.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: <http://www.wias-berlin.de/>

Abstract

We propose a fast method for high order approximations of the solution of n -dimensional parabolic problems over hyper-rectangular domains in the framework of the method of approximate approximations. This approach, combined with separated representations, makes our method effective also in very high dimensions. We report on numerical results illustrating that our formulas are accurate and provide the predicted approximation rate $\mathcal{O}(\epsilon^k)$ also in high dimensions.

1 Introduction

Multidimensional boundary value problems arise in mathematical physics, financial mathematics, biology, chemistry and other applied fields. The computational complexity of the algorithms grows exponentially in the dimension. This effect was called "curse of dimensionality"(Bellmann) and it was the greatest impediment to solving real-world problems.

In [6] and [7], Beylkin and Mohlenkamp introduced the strategy of "Separated representations"(also tensor structured approximations) which allowed to perform numerical computations in higher dimensions. In recent years modern methods based on tensor product approximations have been applied successfully (e.g. [2, 3, 5, 9, 11, 12, 13, 15] and the references therein) to some class of multidimensional integral operators.

Some algorithms approximate the operator kernel by a linear combination of exponentials or Gaussians leading to a tensor product approximation. Other methods are based on piecewise polynomial approximations of a separated representation of the density. Then the integral operator applied to the basis functions is approximated by computing a number of one-dimensional integrals.

A different method with high accuracy, which does not approximate or modify the kernel of the integral operator, was introduced in [16] and [18] for the cubature of high dimensional Newton potential over the full space and over half spaces. Here the integral density is approximated by basis functions introduced in the method of approximate approximations, which provides high order semi-analytic cubature formulas. This approach, combined with separated representations, makes the method fast and effective also in very high dimensions. The new approach can be generalized to potentials of other elliptic differential operators acting on densities on hyper-rectangular domains. In [17] and, more generally, in [19], a corresponding cubature method was introduced for stationary advection-diffusion equations, which provides very efficiently high order approximations.

In this paper we show that our approach can be extended to parabolic problems. We propose a fast method in the framework of approximate approximations for the n -dimensional time dependent problem

$$\begin{aligned} \frac{\partial u}{\partial t} - \Delta_{\mathbf{x}}u + 2\mathbf{b} \cdot \nabla_{\mathbf{x}}u + cu &= f(\mathbf{x}, t), \\ u(\mathbf{x}, 0) &= g(\mathbf{x}) \end{aligned} \tag{1.1}$$

for $(\mathbf{x}, t) \in \mathbb{R}^n \times \mathbb{R}_+$ with $\mathbb{R}_+ = [0, \infty)$, $\mathbf{b} \in \mathbb{C}^n$, $c \in \mathbb{C}$. We suppose that f and g are supported with respect to \mathbf{x} in a hyper-rectangle $[\mathbf{P}, \mathbf{Q}] = \{\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n : P_j \leq x_j \leq Q_j, j = 1, \dots, n\}$,

$\text{supp } f \subseteq [\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+$, $\text{supp } g \subseteq [\mathbf{P}, \mathbf{Q}]$. The solution of (1.1) can be written as [8, p. 49]

$$u(\mathbf{x}, t) = \mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f(\mathbf{x}, t) + \mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} g(\mathbf{x}, t), \quad (1.2)$$

where

$$\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} g(\mathbf{x}, t) = \frac{e^{-ct}}{(4\pi t)^{n/2}} \int_{[\mathbf{P}, \mathbf{Q}]} e^{-|\mathbf{x}-\mathbf{y}-2\mathbf{b}t|^2/(4t)} g(\mathbf{y}) d\mathbf{y}, \quad (1.3)$$

$$\begin{aligned} \mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f(\mathbf{x}, t) &= \int_0^t \frac{e^{-cs} ds}{(4\pi s)^{n/2}} \int_{[\mathbf{P}, \mathbf{Q}]} e^{-|\mathbf{x}-\mathbf{y}-2\mathbf{b}s|^2/(4s)} f(\mathbf{y}, t-s) d\mathbf{y} \\ &= \int_0^t (\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f(\cdot, s))(\mathbf{x}, t-s) ds. \end{aligned} \quad (1.4)$$

Our method consists in approximating the functions f and g via the basis functions introduced by approximate approximations, which are product of Gaussians and special polynomials. The action of the potential $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})}$ applied to the basis functions admits a separated representation, i.e., it is represented as product of functions depending only on one of the space variables. Then a separated representation of the initial condition g (see (2.9)) provides a separated representation of the potential. Moreover, the action of $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})}$ on the basis functions allows for one-dimensional integral representations with separated integrands. This construction, combined with an accurate quadrature rule as suggested in [22] and a separated representation of the density f , provides a separated representation of the integral operator (1.4). Thus for the computation of (1.1) only one-dimensional operations are used. We derive formulas of an arbitrary high order, fast and accurate also in high dimensions. The accuracy of the method and the convergence orders 2, 4 and 6 are confirmed by numerical experiments.

The paper is organized as follows. We start in section 2 by describing the method in the case of second order approximations. We then consider higher order approximations in section 3 and, for f and g with separated representation, we derive a tensor product representation of $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f$ and $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} g$ which admits efficient one-dimensional operations. Finally, in section 4, we report on numerical results, illustrating that our formulas are accurate and provide the predicted approximation rates 2, 4 and 6 also if the dimension is high.

2 Description of the method

In this section we describe the basic algorithm. First, we introduce approximate quasi-interpolants and describe their use to approximate f and g in (1.1). Second, we show how that formulas are used to obtain approximation formulas for the solution of (1.1). Third, for densities f and g with separated representation, we derive a tensor product representation for the integral operators $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f$ and $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} g$.

2.1 Approximate quasi-interpolants

The method of approximate approximations consists in approximating the function f and g in (1.1) by

quasi-interpolants on the rectangular grids $\{(h\mathbf{m}, \tau i)\}$ and $\{h\mathbf{m}\}$, respectively,

$$\mathcal{M}_{h,\tau}f(\mathbf{x}, t) = \frac{1}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{i \in \mathbb{Z} \\ \mathbf{m} \in \mathbb{Z}^n}} f(h\mathbf{m}, \tau i) \tilde{\eta} \left(\frac{t - \tau i}{\tau\sqrt{\mathcal{D}_0}} \right) \eta \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}} \right), \quad (2.1)$$

$$\mathcal{N}_hg(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{D}^n}} \sum_{\mathbf{m} \in \mathbb{Z}^n} g(h\mathbf{m}) \eta \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}} \right). \quad (2.2)$$

Here τ and h are the steps; \mathcal{D}_0 and \mathcal{D} are positive fixed parameters; $\tilde{\eta} \in \mathcal{S}(\mathbb{R})$ and $\eta \in \mathcal{S}(\mathbb{R}^n)$ are the generating functions, which belong to the Schwartz space \mathcal{S} of smooth and rapidly decaying functions.

We say that the generating functions fulfill the moment condition of order N_0 and N , respectively, if

$$\int_{\mathbb{R}} \tilde{\eta}(t) t^s dt = \delta_{0,s}, \quad 0 \leq s < N_0; \quad \int_{\mathbb{R}^n} \eta(\mathbf{x}) \mathbf{x}^\alpha d\mathbf{x} = \delta_{0,\alpha}, \quad 0 \leq |\alpha| < N. \quad (2.3)$$

The main feature of the approximate quasi-interpolation is expressed in the following

Theorem 2.1. ([21, p. 34]) *Suppose that the generating functions satisfy conditions (2.3). Given $\varepsilon > 0$ there exist $\mathcal{D} > 0$ and $\mathcal{D}_0 > 0$ such that, for any $f \in C_0^L(\mathbb{R}^n \times \mathbb{R})$ with $L = \max(N, N_0)$ and $g \in C_0^N(\mathbb{R}^n)$, the approximation errors of the quasi-interpolants (2.1), (2.2) can be estimated pointwise by*

$$\begin{aligned} |f(\mathbf{x}, t) - \mathcal{M}_{h,\tau}f(\mathbf{x}, t)| &\leq c_1(h\sqrt{\mathcal{D}})^N + c_2(\tau\sqrt{\mathcal{D}_0})^{N_0} \\ &+ \varepsilon \left(\sum_{|\alpha|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\alpha|}}{\alpha!} \|\partial_{\mathbf{x}}^\alpha f\|_{L^\infty} + \sum_{s=0}^{N_0-1} \frac{(\tau\sqrt{\mathcal{D}_0})^s}{s!} \|\partial_t^s f\|_{L^\infty} \right), \quad (2.4) \\ |g(\mathbf{x}) - \mathcal{N}_hg(\mathbf{x})| &\leq c_1(h\sqrt{\mathcal{D}})^N + \varepsilon \sum_{|\alpha|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\alpha|}}{\alpha!} \|\partial_{\mathbf{x}}^\alpha g\|_{L^\infty}, \end{aligned}$$

where the constants c_1 and c_2 do not depend on $h, \tau, \mathcal{D}, \mathcal{D}_0$.

To construct an approximate solution of (1.1) we approximate f and g such that the integrals $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)}$ and $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)}$ applied to it can be computed, analytically or at least efficiently. This can be done if g in $[\mathbf{P}, \mathbf{Q}]$ and f in $[\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+$ are approximated by quasi-interpolants (2.1), (2.2) with appropriately chosen generating functions.

The functions g and f are C^N with respect to \mathbf{x} in $[\mathbf{P}, \mathbf{Q}]$, but vanish for $\mathbf{x} \notin [\mathbf{P}, \mathbf{Q}]$. Thus the sum

$$\frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in [\mathbf{P}, \mathbf{Q}]} g(h\mathbf{m}) \eta \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}} \right)$$

approximates g only in a subdomain of $[\mathbf{P}, \mathbf{Q}]$, similarly

$$\frac{1}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{(h\mathbf{m}, \tau i) \in [\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+} f(h\mathbf{m}, \tau i) \tilde{\eta} \left(\frac{t - \tau i}{\tau\sqrt{\mathcal{D}_0}} \right) \eta \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}} \right)$$

approximates \tilde{f} only in a subdomain of $[\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+$. Therefore we extend g and f into a larger domain with preserved smoothness such that the extensions \tilde{g} and \tilde{f} satisfy

$$\|\tilde{g}\|_{W_\infty^N(\mathbb{R}^n)} \leq C\|g\|_{W_\infty^N([\mathbf{P}, \mathbf{Q}])}, \quad \|\tilde{f}\|_{W_\infty^L(\mathbb{R}^n \times \mathbb{R})} \leq C\|f\|_{W_\infty^L([\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+)}, \quad C > 0.$$

The quasi-interpolants of the extensions \tilde{f} and \tilde{g} approximate f in $[\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+$ and g in $[\mathbf{P}, \mathbf{Q}]$ with the error estimate (2.4). The extensions can be done, for example, by using Hestenes reflection principle ([14], see also [20, p. 27]). This is considered in section 4.

Since η and $\tilde{\eta}$ are smooth and of rapid decay, for any error $\varepsilon > 0$ one can fix $r > 0$, $r_0 > 0$ and positive parameters \mathcal{D} and \mathcal{D}_0 such that the quasi-interpolants

$$\begin{aligned} \mathcal{M}_{h,\tau}^{(r)} f(\mathbf{x}, t) &= \frac{1}{\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0 \tau} \\ h\mathbf{m} \in \Omega_{rh}}} \tilde{f}(h\mathbf{m}, \tau i) \tilde{\eta}\left(\frac{t - \tau i}{\tau \sqrt{\mathcal{D}_0}}\right) \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right), \\ \mathcal{N}_h^{(r)} g(\mathbf{x}) &= \frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right), \end{aligned}$$

provide the error estimates

$$\begin{aligned} |f(\mathbf{x}, t) - \mathcal{M}_{h,\tau}^{(r)} f(\mathbf{x}, t)| &= \mathcal{O}((h\sqrt{\mathcal{D}})^N + (\tau\sqrt{\mathcal{D}_0})^{N_0}) + \varepsilon, \\ |g(\mathbf{x}) - \mathcal{N}_h^{(r)} g(\mathbf{x})| &= \mathcal{O}((h\sqrt{\mathcal{D}})^N) + \varepsilon \end{aligned} \quad (2.5)$$

for all $\mathbf{x} \in [\mathbf{P}, \mathbf{Q}]$ and $t \in [0, T]$, $T > 0$. Here $\tilde{\Omega}_{r_0 \tau} = (-r_0 \tau \sqrt{\mathcal{D}_0}, T + r_0 \tau \sqrt{\mathcal{D}_0})$ and $\Omega_{rh} = \prod_{j=1}^n I_j$ with $I_j = (P_j - rh\sqrt{\mathcal{D}}, Q_j + rh\sqrt{\mathcal{D}})$.

2.2 Approximation of the solution (1.2)

Cubature formulas for (1.3) and (1.4) are derived by replacing the densities g and f with the quasi-interpolants $\mathcal{N}_h^{(r)} g$ and $\mathcal{M}_{h,\tau}^{(r)} f$. Then the sum

$$\begin{aligned} \mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)}(\mathcal{N}_h^{(r)} g)(\mathbf{x}, t) &= \frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \frac{e^{-ct}}{(4\pi t)^{n/2}} \int_{[\mathbf{P}, \mathbf{Q}]} e^{-|\mathbf{x}-\mathbf{y}-2bt|^2/(4t)} \eta\left(\frac{\mathbf{y} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right) d\mathbf{y} \\ &= \frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C,B)} \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{t}{h^2 \mathcal{D}}\right) \end{aligned}$$

with $C = h^2 \mathcal{D} c$, $\mathbf{B} = h\sqrt{\mathcal{D}} \mathbf{b}$, $\mathbf{P}_m = (\mathbf{P} - h\mathbf{m})/(h\sqrt{\mathcal{D}})$ and $\mathbf{Q}_m = (\mathbf{Q} - h\mathbf{m})/(h\sqrt{\mathcal{D}})$ provides an approximation of $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)} g(\mathbf{x}, t)$ in $[\mathbf{P}, \mathbf{Q}] \times [0, T]$. Similarly,

$$\begin{aligned} \mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)}(\mathcal{M}_{h,\tau}^{(r)} f)(\mathbf{x}, t) &= \frac{1}{\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0 \tau} \\ h\mathbf{m} \in \Omega_{rh}}} \tilde{f}(h\mathbf{m}, \tau i) \int_0^t \tilde{\eta}\left(\frac{s - \tau i}{\tau \sqrt{\mathcal{D}_0}}\right) \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C,B)} \eta\left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{t - s}{h^2 \mathcal{D}}\right) ds \end{aligned}$$

approximates $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)} f(\mathbf{x}, t)$ in $[\mathbf{P}, \mathbf{Q}] \times [0, T]$. Denoting

$$u_{h,\tau}(\mathbf{x}, t) = \mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)}(\mathcal{M}_{h,\tau}^{(r)} f)(\mathbf{x}, t) + \mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c,b)}(\mathcal{N}_h^{(r)} g)(\mathbf{x}, t), \quad (2.6)$$

it is easy to deduce the following

Theorem 2.2. For any $\epsilon > 0$ there exist $\mathcal{D} > 0$ and $\mathcal{D}_0 > 0$ such that $u_{h,\tau}$ in (2.6) approximates the solution of the Cauchy problem (1.1) with the error estimate

$$|u(\mathbf{x}, t) - u_{h,\tau}(\mathbf{x}, t)| \leq c_{1,T}(h\sqrt{\mathcal{D}})^N + c_{2,T}(\tau\sqrt{\mathcal{D}_0})^{N_0} + \epsilon \left(\sum_{|\alpha|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\alpha|}}{\alpha!} (\|\partial_{\mathbf{x}}^\alpha g\|_{L^\infty} + \|\partial_{\mathbf{x}}^\alpha f\|_{L^\infty}) + \sum_{s=0}^{N_0-1} \frac{(\tau\sqrt{\mathcal{D}_0})^s}{s!} \|\partial_t^s f\|_{L^\infty} \right),$$

for all $(\mathbf{x}, t) \in \mathbb{R}^n \times [0, T]$. The constants $c_{1,T}$ and $c_{2,T}$ depend only on N and N_0 .

Consider, for example, the generating functions $\eta_2(\mathbf{x}) = e^{-|\mathbf{x}|^2/\pi^{n/2}}$ and $\tilde{\eta}_2(t) = e^{-t^2/\sqrt{\pi}}$. Then the conditions of Theorem 2.1 are fulfilled with $N = N_0 = 2$. Hence, from (2.6), at the points of the uniform grid $\{(h\mathbf{k}, \tau\ell)\}$,

$$u_{h,\tau}(h\mathbf{k}, \tau\ell) = \frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{r_h}} \tilde{g}(h\mathbf{m}) \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{h^2\mathcal{D}} \right) + \frac{1}{\sqrt{\pi\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0\tau} \\ h\mathbf{m} \in \Omega_{r_h}}} \tilde{f}(h\mathbf{m}, \tau i) \int_0^{\tau\ell} e^{-\frac{(\sigma - \tau(\ell-i))^2}{\tau^2\mathcal{D}_0}} \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\sigma}{h^2\mathcal{D}} \right) d\sigma. \quad (2.7)$$

It can be easily seen that from (1.3)

$$\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} \eta_2(\mathbf{x}, t) = e^{-ct} \prod_{j=1}^n (\phi_{P_j}^{(b_j)}(x_j, t) - \phi_{Q_j}^{(b_j)}(x_j, t)) \quad (2.8)$$

with the analytic expression

$$\phi_P^{(b)}(x, t) = \frac{e^{-(x-2bt)^2/(1+4t)}}{2\sqrt{\pi}\sqrt{1+4t}} \operatorname{erfc} \left(\sqrt{\frac{1+4t}{4t}} \left(P - \frac{x-2bt}{1+4t} \right) \right).$$

Here erfc denotes the complementary error function ([1, p. 262])

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt.$$

Using the idea of approximate approximations, cubature formulas for the Poisson integral (1.3) were constructed in [21, p. 120]. However, due to the number of operations which grows exponentially in n , these formulas are practical only for $n \leq 3$.

2.3 Tensor product formulas

The computation of the convolutions in (2.7) is very efficient if the functions $\tilde{g}(\mathbf{x})$ and $\tilde{f}(\mathbf{x}, t)$ allow a separated representation; that is, within a prescribed accuracy ϵ , they can be represented as sum of products of univariate functions

$$\tilde{g}(\mathbf{x}) = \sum_{p=1}^P \alpha_p \prod_{j=1}^n g_j^{(p)}(x_j) + \mathcal{O}(\epsilon), \quad \tilde{f}(\mathbf{x}, t) = \sum_{p=1}^P \beta_p \prod_{j=1}^n f_j^{(p)}(x_j, t) + \mathcal{O}(\epsilon) \quad (2.9)$$

with suitable functions $g_j^{(p)}$ and $f_j^{(p)}$, chosen such that the separation rank P is small. Low-rank separated representations have been studied for many years and various approaches have been proposed (see [10, 2.7] and the references therein). The class of functions that can be approximated accurately with small P is wide enough to include important examples of functions of many variables, and so the methods are useful in practice and allow algorithms that scales linearly in n [4].

Let us denote the two sums on the right in (2.7) by Σ_1 and Σ_2 . Then Σ_1 is approximated by the product of one-dimensional sums

$$\Sigma_1 = \frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{h^2\mathcal{D}} \right) \approx \frac{e^{-c\tau\ell}}{\mathcal{D}^{n/2}} \sum_{p=1}^P \alpha_p \prod_{j=1}^n S_j^{(p)}(k_j, \tau\ell)$$

where

$$S_j^{(p)}(k_j, t) = \sum_{hm_j \in I_j} g_j^{(p)}(hm_j) \left(\phi_{P_{m_j}}^{(h\sqrt{\mathcal{D}}b_j)} \left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}}, \frac{t}{h^2\mathcal{D}} \right) - \phi_{Q_{m_j}}^{(h\sqrt{\mathcal{D}}b_j)} \left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}}, \frac{t}{h^2\mathcal{D}} \right) \right).$$

Here we set

$$P_{m_j} = \frac{P_j - hm_j}{h\sqrt{\mathcal{D}}}, \quad Q_{m_j} = \frac{Q_j - hm_j}{h\sqrt{\mathcal{D}}}.$$

The second term Σ_2 involves additionally an integration

$$K_2(h\mathbf{k}, h\mathbf{m}, \tau\ell, \tau i) = \int_0^{\tau\ell} e^{-(\tau\ell - \sigma - \tau i)^2 / (\tau^2 \mathcal{D}_0)} \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\sigma}{h^2\mathcal{D}} \right) d\sigma,$$

which cannot be taken analytically. Therefore we use an efficient quadrature based on the classical trapezoidal rule, which is exponentially converging for rapidly decaying smooth functions on the real line (see [23, 22]). Making the substitution

$$\sigma = \frac{\tau\ell}{2} \left(1 + \tanh \left(\frac{\pi}{2} \sinh \xi \right) \right) = \frac{\tau\ell}{1 + e^{-\pi \sinh \xi}}, \quad (2.10)$$

introduced in [22], K_2 transforms to the following integral over \mathbb{R} with doubly exponentially decaying integrand

$$\begin{aligned} & K_2(h\mathbf{k}, h\mathbf{m}, \tau\ell, \tau i) \\ &= \frac{\pi\tau\ell}{2} \int_{-\infty}^{\infty} \frac{e^{-(\ell/(1+e^{\pi \sinh \xi}) - i)^2 / \mathcal{D}_0} \cosh \xi}{1 + \cosh(\pi \sinh \xi)} \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{h^2\mathcal{D}(1 + e^{-\pi \sinh \xi})} \right) d\xi. \end{aligned}$$

The trapezoidal rule with step size κ gives for sufficiently large $S \in \mathbb{N}$

$$K_2(h\mathbf{k}, h\mathbf{m}, \tau\ell, \tau i) \approx \frac{\pi\tau\ell\kappa}{2} \sum_{s=-S}^S \omega_s e^{-(\ell/(1+e^{\pi \sinh(s\kappa)}) - i)^2 / \mathcal{D}_0} \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{a_s h^2\mathcal{D}} \right)$$

where we denote

$$\omega_s = \frac{\cosh(s\kappa)}{1 + \cosh(\pi \sinh(s\kappa))}, \quad a_s = 1 + e^{-\pi \sinh(s\kappa)}. \quad (2.11)$$

Then for Σ_2 one gets

$$\Sigma_2 \approx \frac{\tau \ell \kappa \sqrt{\pi}}{2\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{s=-S}^S \omega_s \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0 \tau} \\ h\mathbf{m} \in \Omega_{rh}}} e^{-\ell/(1+e^{\pi \sinh(s\kappa)})-i)^2/\mathcal{D}_0} \tilde{f}(h\mathbf{m}, \tau i) \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau \ell}{a_s h^2 \mathcal{D}} \right).$$

By using the separate representation (2.9) of \tilde{f} and (2.8) we can approximate similar to Σ_1

$$\sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{f}(h\mathbf{m}, \tau i) \mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \eta_2 \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau \ell}{a_s h^2 \mathcal{D}} \right) \approx e^{-c\tau \ell / a_s} \sum_{p=1}^P \beta_p \prod_{j=1}^n T_j^{(p)}(k_j, \tau \ell, \tau i, a_s),$$

where

$$T_j^{(p)}(k_j, \tau \ell, \tau i, a_s) = \sum_{hm_j \in I_j} f_j^{(p)}(hm_j, \tau i) \times \left(\phi_{P_{m_j}}^{(h\sqrt{\mathcal{D}}b_j)} \left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}}, \frac{\tau \ell}{a_s h^2 \mathcal{D}} \right) - \phi_{Q_{m_j}}^{(h\sqrt{\mathcal{D}}b_j)} \left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}}, \frac{\tau \ell}{a_s h^2 \mathcal{D}} \right) \right).$$

Thus we get the efficiently computable second order approximation (2.7) of the initial value problem (1.1)

$$u_{h,\tau}(h\mathbf{k}, \tau \ell) \approx \frac{e^{-c\tau \ell}}{\mathcal{D}^{n/2}} \sum_{p=1}^P \alpha_p \prod_{j=1}^n S_j^{(p)}(k_j, \tau \ell) + \frac{\tau \ell \kappa \sqrt{\pi}}{2\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{s=-S}^S \omega_s e^{-c\tau \ell / a_s} \sum_{\tau i \in \tilde{\Omega}_{r_0 \tau}} e^{-\ell/(1+e^{\pi \sinh(s\kappa)})-i)^2/\mathcal{D}_0} \sum_{p=1}^P \beta_p \prod_{j=1}^n T_j^{(p)}(k_j, \tau \ell, \tau i, a_s). \quad (2.12)$$

In the following we show that the same ideas hold also for higher order approximations.

3 High order cubature formulas

We assume that $\eta(\mathbf{x})$ is the product of univariate basis functions of the form Gaussians times special polynomials

$$\eta(\mathbf{x}) = \prod_{j=1}^n \eta_{2M}(x_j); \quad \eta_{2M}(x_j) = \frac{(-1)^{M-1}}{2^{2M-1} \sqrt{\pi} (M-1)!} \frac{H_{2M-1}(x_j) e^{-x_j^2}}{x_j}, \quad (3.1)$$

where H_k are the Hermite polynomials

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

and $\tilde{\eta}(t) = \eta_{2M_0}(t)$. The functions $\tilde{\eta}$ and η satisfy the moment conditions of order $N_0 = 2M_0$ and $N = 2M$, respectively (cf. [21, p. 56]).

To get formulas similar to (2.12) for higher order approximations, we approximate the density with quasi-interpolants based on (3.1). We start with the following

Theorem 3.1. Let $M \geq 1$. The integral (1.3) applied to the generating function $\prod_{j=1}^n \eta_{2M}(x_j)$ in (3.1) can be written as

$$(\mathcal{P}_{[P,Q]}^{(c,b)}(\prod_{j=1}^n \eta_{2M}(\cdot)))(\mathbf{x}, t) = e^{-ct} \prod_{j=1}^n (\Phi_M(4t, x_j - 2b_j t, P_j) - \Phi_M(4t, x_j - 2b_j t, Q_j)) \quad (3.2)$$

where

$$\Phi_M(t, x, p) = \frac{e^{-x^2/(1+t)}}{2\sqrt{\pi}} \left(\operatorname{erfc}(F(t, x, p)) \mathcal{R}_M(t, x) - \frac{e^{-F^2(t, x, p)}}{\sqrt{\pi}} \mathcal{Q}_M(t, x, p) \right),$$

with

$$\begin{aligned} F(t, x, p) &= \sqrt{\frac{1+t}{t}} \left(p - \frac{x}{1+t} \right), \\ \mathcal{R}_M(t, x) &= \sum_{k=0}^{M-1} \frac{1}{(1+t)^{k+1/2}} \frac{(-1)^k}{4^k k!} H_{2k} \left(\frac{x}{\sqrt{1+t}} \right), \\ \mathcal{Q}_1(t, x, p) &= 0, \\ \mathcal{Q}_M(t, x, p) &= 2 \sum_{k=1}^{M-1} \frac{(-1)^k}{k! 4^k} \sum_{\ell=1}^{2k} \frac{(-1)^\ell}{t^{\ell/2}} \left(H_{2k-\ell}(p) H_{\ell-1} \left(\frac{p-x}{\sqrt{t}} \right) \right. \\ &\quad \left. - \binom{2k}{\ell} H_{2k-\ell} \left(\frac{x}{\sqrt{1+t}} \right) \frac{H_{\ell-1}(F(t, x, p))}{(1+t)^{k+1/2}} \right), \quad M > 1. \end{aligned}$$

\mathcal{R}_M and \mathcal{Q}_M are polynomials in x of degree $2M-2$ and $2M-3$ (provided that $M > 1$), respectively.

Proof. The computation of the integral (1.3) applied to a generating function with tensor product form is reduced to the computation of one-dimensional integrals

$$(\mathcal{P}_{[P,Q]}^{(c,b)}(\prod_{j=1}^n \eta_{2M}(\cdot)))(\mathbf{x}, \frac{t}{4}) = e^{-ct/4} \prod_{j=1}^n \frac{1}{\sqrt{\pi t}} \int_{P_j}^{Q_j} e^{-(x_j - b_j t/2 - y_j)^2/t} \eta_{2M}(y_j) dy_j.$$

Using the representation ([21, p. 55])

$$\eta_{2M}(y) = \frac{1}{\sqrt{\pi}} \sum_{j=0}^{M-1} \frac{(-1)^j}{j! 4^j} \frac{\partial^{2j}}{\partial y^{2j}} e^{-y^2}$$

we have proved in [17, Theorem 1], that

$$\frac{1}{\sqrt{\pi t}} \int_p^\infty e^{-(x-y)^2/t} \eta_{2M}(y) dy = \Phi_M(t, x, p),$$

and (3.2) follows. □

For $M = 1, 2, 3$ the functions \mathcal{R}_M and \mathcal{Q}_M are given by

$$\begin{aligned}\mathcal{R}_1(t, x) &= \frac{1}{\sqrt{1+t}}; & \mathcal{Q}_1(t, x, p) &= 0, \\ \mathcal{R}_2(t, x) &= \mathcal{R}_1(t, x) + \frac{1}{2(1+t)^{3/2}} - \frac{x^2}{(1+t)^{5/2}}, & \mathcal{Q}_2(t, x, p) &= \frac{\sqrt{t}}{(1+t)} \left(\frac{x}{1+t} + p \right), \\ \mathcal{R}_3(t, x) &= \mathcal{R}_2(t, x) + \frac{3}{8(1+t)^{5/2}} - \frac{3x^2}{2(1+t)^{7/2}} + \frac{x^4}{2(1+t)^{9/2}}, \\ \mathcal{Q}_3(t, x, p) &= -\frac{\sqrt{t}}{4(1+t)} \left(\frac{2x^3}{(1+t)^3} + \frac{2px^2 - 5x}{(1+t)^2} + \frac{(2p^2 - 5)x - 3p}{1+t} + p(2p^2 - 7) \right).\end{aligned}$$

Using Theorem 3.1, we can specify the high order approximation

$$\begin{aligned}\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})}(\mathcal{N}_h^{(r)} g)(\mathbf{x}, t) &= \frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \left(\mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \prod_{j=1}^n \eta_{2M}(\cdot) \right) \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{t}{h^2\mathcal{D}} \right) \\ &= \frac{e^{-ct}}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \prod_{j=1}^n \left(\Phi_M \left(\frac{4t}{h^2\mathcal{D}}, \frac{x_j - hm_j - 2b_j t}{h\sqrt{\mathcal{D}}}, P_{m_j} \right) \right. \\ &\quad \left. - \Phi_M \left(\frac{4t}{h^2\mathcal{D}}, \frac{x_j - hm_j - 2b_j t}{h\sqrt{\mathcal{D}}}, Q_{m_j} \right) \right)\end{aligned}$$

for the generating function η defined in (3.1). This is a semi-analytic cubature formula for $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} g(\mathbf{x}, t)$ with the error $\mathcal{O}((h\sqrt{\mathcal{D}})^{2M})$. If additionally \tilde{g} allows a separated representation

$$\tilde{g}(\mathbf{x}) \approx \sum_{p=1}^P \alpha_p \prod_{j=1}^n g_j^{(p)}(x_j), \quad (3.3)$$

then we derive at the points of the uniform grid $\{(h\mathbf{k}, \tau\ell)\}$

$$\frac{1}{\mathcal{D}^{n/2}} \sum_{h\mathbf{m} \in \Omega_{rh}} \tilde{g}(h\mathbf{m}) \left(\mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \prod_{j=1}^n \eta_{2M}(\cdot) \right) \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{h^2\mathcal{D}} \right) \approx \frac{e^{-c\tau\ell}}{\mathcal{D}^{n/2}} \sum_{p=1}^P \alpha_p \prod_{j=1}^n S_j^{(p)}(k_j, \tau\ell)$$

where now

$$\begin{aligned}S_j^{(p)}(k_j, t) &= \\ &\sum_{hm_j \in I_j} g_j^{(p)}(hm_j) \left(\Phi_M \left(\frac{4t}{h^2\mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j t}{h\sqrt{\mathcal{D}}}, P_{m_j} \right) - \Phi_M \left(\frac{4t}{h^2\mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j t}{h\sqrt{\mathcal{D}}}, Q_{m_j} \right) \right).\end{aligned}$$

Similarly, we specify the approximation

$$\begin{aligned}\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})}(\mathcal{M}_{h, \tau}^{(r)} f)(\mathbf{x}, t) &= \\ &\frac{1}{\sqrt{\mathcal{D}_0} \mathcal{D}^n} \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0 \tau} \\ h\mathbf{m} \in \Omega_{rh}}} \tilde{f}(h\mathbf{m}, \tau i) \int_0^t \eta_{2M_0} \left(\frac{s - \tau i}{\tau \sqrt{\mathcal{D}_0}} \right) \left(\mathcal{P}_{[\mathbf{P}_m, \mathbf{Q}_m]}^{(C, \mathbf{B})} \prod_{j=1}^n \eta_{2M}(\cdot) \right) \left(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{t - s}{h^2\mathcal{D}} \right) ds.\end{aligned}$$

At the points $\{(h\mathbf{k}, \tau\ell)\}$ we have

$$\begin{aligned} & \mathcal{H}_{[P,Q]}(\mathcal{M}_{h,\tau}^{(\tau)} f)(h\mathbf{k}, \tau\ell) \\ &= \frac{1}{\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0 \tau} \\ h\mathbf{m} \in \Omega_{rh}}} \tilde{f}(h\mathbf{m}, \tau i) \int_0^{\tau\ell} \eta_{2M_0} \left(\frac{\tau\ell - \sigma - \tau i}{\tau\sqrt{\mathcal{D}_0}} \right) \left(\mathcal{P}_{[P_{\mathbf{m}}, Q_{\mathbf{m}}]}^{(C,B)} \prod_{j=1}^n \eta_{2M}(\cdot) \right) \left(\frac{\mathbf{k} - \mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{\sigma}{h^2 \mathcal{D}} \right) d\sigma \\ &= \frac{1}{\sqrt{\pi \mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{\tau i \in \tilde{\Omega}_{r_0 \tau} \\ h\mathbf{m} \in \Omega_{rh}}} \tilde{f}(h\mathbf{m}, \tau i) K_{M, M_0}(h\mathbf{k}, h\mathbf{m}, \tau\ell, \tau i) \end{aligned}$$

where, in view of (3.1) and Theorem 3.1

$$\begin{aligned} K_{M, M_0}(h\mathbf{k}, h\mathbf{m}, \tau\ell, \tau i) &= \frac{(-1)^{M_0-1} \tau \sqrt{\mathcal{D}_0}}{2^{2M_0-1} (M_0-1)!} \int_0^{\tau\ell} \frac{e^{-c\sigma} e^{-(\tau\ell - \sigma - \tau i)^2 / (\tau^2 \mathcal{D}_0)}}{\tau\ell - \sigma - \tau i} H_{2M_0-1} \left(\frac{\tau\ell - \sigma - \tau i}{\tau\sqrt{\mathcal{D}_0}} \right) \\ &\quad \times \prod_{j=1}^n \left(\Phi_M \left(\frac{4\sigma}{h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \sigma}{h\sqrt{\mathcal{D}}}, P_{\mathbf{m}_j} \right) - \Phi_M \left(\frac{4\sigma}{h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \sigma}{h\sqrt{\mathcal{D}}}, Q_{\mathbf{m}_j} \right) \right) d\sigma. \end{aligned}$$

Again, by making the substitution (2.10), the integrals are transformed to

$$\begin{aligned} & \frac{(-1)^{M_0-1} \pi \tau \ell \sqrt{\mathcal{D}_0}}{2^{2M_0} (M_0-1)!} \int_{-\infty}^{\infty} \frac{e^{-(\ell/(1+e^{\pi \sinh \xi}) - i)^2 / \mathcal{D}_0} e^{-c\tau\ell/(1+e^{-\pi \sinh \xi})}}{\ell/(1+e^{\pi \sinh \xi}) - i} H_{2M_0-1} \left(\frac{\ell/(1+e^{\pi \sinh \xi}) - i}{\sqrt{\mathcal{D}_0}} \right) \\ & \quad \times \frac{\cosh \xi}{1 + \cosh(\pi \sinh \xi)} \prod_{j=1}^n \left(\Phi_M \left(\frac{4\tau\ell}{h^2 \mathcal{D} (1 + e^{-\pi \sinh \xi})}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \tau\ell}{h\sqrt{\mathcal{D}} (1 + e^{-\pi \sinh \xi})}, P_{\mathbf{m}_j} \right) \right. \\ & \quad \left. - \Phi_M \left(\frac{4\tau\ell}{h^2 \mathcal{D} (1 + e^{-\pi \sinh \xi})}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \tau\ell}{h\sqrt{\mathcal{D}} (1 + e^{-\pi \sinh \xi})}, Q_{\mathbf{m}_j} \right) \right) d\xi \end{aligned}$$

with integrands decaying doubly exponentially. Then the trapezoidal rule with step size κ and $S \in \mathbb{N}$ gives

$$\begin{aligned} & K_{M, M_0}(h\mathbf{k}, h\mathbf{m}, \tau\ell, \tau i) \\ & \approx \frac{(-1)^{M_0-1} \pi \tau \ell \kappa \sqrt{\mathcal{D}_0}}{2^{2M_0} (M_0-1)!} \sum_{s=-S}^S e^{-c\tau\ell/a_s} \frac{e^{-(\ell/(1+e^{\pi \sinh(\kappa s)}) - i)^2 / \mathcal{D}_0}}{\ell/(1+e^{\pi \sinh(\kappa s)}) - i} H_{2M_0-1} \left(\frac{\ell/(1+e^{\pi \sinh(\kappa s)}) - i}{\sqrt{\mathcal{D}_0}} \right) \\ & \quad \times \omega_s \prod_{j=1}^n \left(\Phi_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \tau\ell}{a_s h \sqrt{\mathcal{D}}}, P_{\mathbf{m}_j} \right) - \Phi_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \tau\ell}{a_s h \sqrt{\mathcal{D}}}, Q_{\mathbf{m}_j} \right) \right) \end{aligned}$$

with ω_s, a_s given in (2.11). By using the separate representation (2.9) of \tilde{f} we derive

$$\begin{aligned} & \mathcal{H}_{[P,Q]}(\mathcal{M}_{h,\tau}^{(\tau)} f)(h\mathbf{k}, \tau\ell) \approx \sqrt{\frac{\pi}{\mathcal{D}^n}} \frac{(-1)^{M_0-1} \tau \ell \kappa}{2^{2M_0} (M_0-1)!} \sum_{s=-S}^S \omega_s e^{-c\tau\ell/a_s} \\ & \quad \sum_{\tau i \in \tilde{\Omega}_{r_0 \tau}} \frac{e^{-(\ell/(1+e^{\pi \sinh(\kappa s)}) - i)^2 / \mathcal{D}_0}}{\ell/(1+e^{\pi \sinh(\kappa s)}) - i} H_{2M_0-1} \left(\frac{\ell/(1+e^{\pi \sinh(\kappa s)}) - i}{\sqrt{\mathcal{D}_0}} \right) \sum_{p=1}^P \beta_p \prod_{j=1}^n T_j^{(p)}(k_j, \tau\ell, \tau i, a_s) \end{aligned}$$

where now the one-dimensional sums $T_j^{(p)}$ are given by

$$T_j^{(p)}(k_j, \tau\ell, \tau i, a_s) = \sum_{hm_j \in I_j} f_j^{(p)}(hm_j, \tau i) \\ \times \left(\Phi_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \tau\ell}{a_s h \sqrt{\mathcal{D}}}, P_{\mathbf{m}_j} \right) - \Phi_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j \tau\ell}{a_s h \sqrt{\mathcal{D}}}, Q_{\mathbf{m}_j} \right) \right).$$

Thus we get a computable approximation of the initial value problem (1.1)

$$u_{h,\tau}(h\mathbf{k}, \tau\ell) \approx \frac{e^{-c\tau\ell}}{\mathcal{D}^{n/2}} \sum_{p=1}^P \alpha_p \prod_{j=1}^n S_j^{(p)}(k_j, \tau\ell) + \\ \frac{\tau\ell\kappa\pi}{2\sqrt{\mathcal{D}_0}\mathcal{D}^n} \sum_{s=-S}^S \omega_s e^{-c\tau\ell/a_s} \sum_{\tau i \in \tilde{\Omega}_{\tau_0\tau}} \eta_{2M_0} \left(\frac{\ell/(1 + e^{\pi \sinh(\kappa s)}) - i}{\sqrt{\mathcal{D}_0}} \right) \sum_{p=1}^P \beta_p \prod_{j=1}^n T_j^{(p)}(k_j, \tau\ell, \tau i, a_s),$$

which has the order $\mathcal{O}((h\sqrt{\mathcal{D}})^{2M} + (\tau\sqrt{\mathcal{D}_0})^{2M_0})$ for $(\mathbf{x}, t) \in \mathbb{R}^n \times [0, T]$, $T > 0$.

3.1 A generalization of problem (1.1)

Consider the initial value problem for the parabolic equation

$$\frac{\partial u}{\partial t} - A \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} u + 2\mathbf{b} \cdot \nabla_{\mathbf{x}} u + c u = f(\mathbf{x}, t) \quad \text{in } \mathbb{R}^n \times \mathbb{R}_+ \quad (3.4)$$

$$u(\mathbf{x}, 0) = g(\mathbf{x}) \quad \text{on } \mathbb{R}^n. \quad (3.5)$$

where the matrix A of order n is supposed to be real, symmetric and positive definite. There exist an orthogonal matrix O and a diagonal matrix D with positive entries such that $A = O^T D^2 O$. By introducing new coordinates $\boldsymbol{\xi} = D^{-1} O \mathbf{x}$ we have $\nabla_{\mathbf{x}} = O^T D^{-1} \nabla_{\boldsymbol{\xi}}$ and $A \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} = \Delta_{\boldsymbol{\xi}}$. Hence, if we set $U(\boldsymbol{\xi}, t) = u(\mathbf{x}, t)$, $F(\boldsymbol{\xi}, t) = f(\mathbf{x}, t)$, $G(\boldsymbol{\xi}) = g(\mathbf{x})$, $\boldsymbol{\beta} = D^{-1} O \mathbf{b}$, then the problem (3.4), (3.5) reduces to the initial value problem

$$\frac{\partial U}{\partial t} - \Delta_{\boldsymbol{\xi}} U + 2\boldsymbol{\beta} \cdot \nabla_{\boldsymbol{\xi}} U + c U = F(\boldsymbol{\xi}, t) \quad \text{in } \mathbb{R}^n \times \mathbb{R}_+ \quad (3.6)$$

$$U(\boldsymbol{\xi}, 0) = G(\boldsymbol{\xi}) \quad \text{on } \mathbb{R}^n. \quad (3.7)$$

The solution of (3.6), (3.7) can be represented as

$$U(\boldsymbol{\xi}, t) = \mathcal{P}^{(c, \boldsymbol{\beta})}(G(\cdot))(\boldsymbol{\xi}, t) + \int_0^t (\mathcal{P}^{(c, \boldsymbol{\beta})} F(\cdot, s))(\boldsymbol{\xi}, t - s) ds \quad (3.8)$$

where

$$\mathcal{P}^{(c, \boldsymbol{\beta})}(f(\cdot))(\boldsymbol{\xi}, t) = \frac{e^{-ct}}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{-|\boldsymbol{\xi} - \mathbf{y} - 2\boldsymbol{\beta}t|^2/(4t)} f(\mathbf{y}) dy.$$

An approximate solution of (3.6), (3.7) can be obtained by using the generating function [21, p. 55] $\eta(\mathbf{x}) = \pi^{-n/2} L_{M-1}^{(n/2)}(|\mathbf{x}|^2) e^{-|\mathbf{x}|^2}$, where $L_j^{(\gamma)}$ are the generalized Laguerre polynomials defined by

$$L_j^{(\gamma)}(y) = \frac{e^y y^{-\gamma}}{k!} \left(\frac{d}{dy} \right)^k (e^{-y} y^{k+\gamma}), \quad \gamma > -1$$

and $\tilde{\eta}(t) = \eta_{2M_0}(t)$ (cf. [21, p. 120]).

In order to get an approximate formula which can be used in high dimensions we use the quasi-interpolants

$$G(\boldsymbol{\xi}) \approx \frac{1}{\mathcal{D}^{n/2}} \sum_{\mathbf{m} \in \mathbb{Z}^n} G(h\mathbf{m}) \prod_{j=1}^n \eta_{2M} \left(\frac{\xi_j - hm_j}{h\sqrt{\mathcal{D}}} \right),$$

$$F(\boldsymbol{\xi}, t) \approx \frac{1}{\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{i \in \mathbb{Z} \\ \mathbf{m} \in \mathbb{Z}^n}} F(h\mathbf{m}, \tau i) \eta_{2M_0} \left(\frac{t - \tau i}{\tau \sqrt{\mathcal{D}_0}} \right) \prod_{j=1}^n \eta_{2M} \left(\frac{\xi_j - hm_j}{h\sqrt{\mathcal{D}}} \right).$$

From (3.8) we obtain the following approximation of U at the nodes $(h\mathbf{k}, \tau\ell)$

$$U_{h,\tau}(h\mathbf{k}, \tau\ell) = \frac{e^{-c\tau\ell}}{(\pi\mathcal{D})^{n/2}} \sum_{\mathbf{m} \in \mathbb{Z}^n} G(h\mathbf{m}) \prod_{j=1}^n \mathcal{P}_M \left(\frac{4\tau\ell}{h^2\mathcal{D}}, \frac{hk_j - hm_j - 2\beta_j\tau\ell}{h\sqrt{\mathcal{D}}} \right)$$

$$+ \frac{1}{\sqrt{\pi^n \mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{i \in \mathbb{Z} \\ \mathbf{m} \in \mathbb{Z}^n}} F(h\mathbf{m}, \tau i) \int_0^{\tau\ell} e^{-c\sigma} \eta_{2M_0} \left(\frac{\tau\ell - \tau i - \sigma}{\tau \sqrt{\mathcal{D}_0}} \right) \prod_{j=1}^n \mathcal{P}_M \left(\frac{4\sigma}{h^2\mathcal{D}}, \frac{hk_j - hm_j - 2\beta_j\sigma}{h\sqrt{\mathcal{D}}} \right) d\sigma,$$

where we denote

$$\mathcal{P}_M(\Theta, \zeta) = e^{-\zeta^2/(1+\Theta)} \mathcal{R}_M(\Theta, \zeta).$$

By making the substitution (2.10), the trapezoidal rule with step size κ provides the quadrature of the integrals

$$\frac{\pi\tau\ell\kappa}{2} \sum_{s=-S}^S \omega_s e^{-c\tau\ell/a_s} \eta_{2M_0} \left(\frac{\ell(1 - 1/a_s) - i}{\sqrt{\mathcal{D}_0}} \right) \prod_{j=1}^n \mathcal{P}_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2\beta_j\tau\ell}{a_s h\sqrt{\mathcal{D}}} \right)$$

with ω_s, a_s given in (2.11). Assuming separated representations

$$G(\boldsymbol{\xi}) = \sum_{p=1}^P \alpha_p \prod_{j=1}^n G_j^{(p)}(\xi_j) + \mathcal{O}(\varepsilon), \quad F(\boldsymbol{\xi}, t) = \sum_{p=1}^P \beta_p \prod_{j=1}^n F_j^{(p)}(\xi_j, t) + \mathcal{O}(\varepsilon),$$

we derive an approximation $u_{h,\tau}(h\mathcal{A}^{-1}\mathbf{k}, \tau\ell) = U_{h,\tau}(h\mathbf{k}, \tau\ell)$ of the solution u of (3.4)

$$u_{h,\tau}(h\mathcal{A}^{-1}\mathbf{k}, \tau\ell) \approx \frac{e^{-c\tau\ell}}{(\pi\mathcal{D})^{n/2}} \sum_{p=1}^P \alpha_p \prod_{j=1}^n \sum_{m_j \in \mathbb{Z}} G_j^{(p)}(hk_j) \mathcal{P}_M \left(\frac{4\tau\ell}{h^2\mathcal{D}}, \frac{hk_j - hm_j - 2\beta_j\tau\ell}{h\sqrt{\mathcal{D}}} \right)$$

$$+ \frac{\pi\tau\ell\kappa}{2\sqrt{\pi^n \mathcal{D}_0 \mathcal{D}^n}} \sum_{s=-S}^S \omega_s e^{-c\tau\ell/a_s} \sum_{i \in \mathbb{Z}} \eta_{2M_0} \left(\frac{\ell(1 - 1/a_s) - i}{\sqrt{\mathcal{D}_0}} \right)$$

$$\times \sum_{p=1}^P \beta_p \prod_{j=1}^n \sum_{m_j \in \mathbb{Z}} F_j^{(p)}(hm_j, \tau i) \mathcal{P}_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2\beta_j\tau\ell}{a_s h\sqrt{\mathcal{D}}} \right).$$

4 Numerical Results

4.1 Initial-value problem

In this section we provide results for the approximation of the solution of the problem

$$\frac{\partial u}{\partial t} - \Delta_{\mathbf{x}} u = 0, \quad (\mathbf{x}, t) \in \mathbb{R}^n \times \mathbb{R}_+; \quad u(\mathbf{x}, 0) = g(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n \quad (4.1)$$

with $\text{supp } g \subseteq [p, q]^n$,

$$g(\mathbf{x}) = \prod_{j=1}^n w(x_j), \quad \mathbf{x} = (x_1, \dots, x_n) \in [p, q]^n \quad (4.2)$$

and $w \in C^N([p, q])$. Then, by using Hestenes reflection principle, we can construct an extension of $w(x)$ outside $[p, q]$ as

$$\tilde{w}(x) = \begin{cases} \sum_{s=1}^{N+1} c_s w(-\alpha_s(x - q) + q), & q < x \leq q + \frac{q-p}{A} \\ w(x), & p \leq x \leq q \\ \sum_{s=1}^{N+1} c_s w(-\alpha_s(x - p) + p), & p - \frac{q-p}{A} \leq x < p \end{cases} \quad (4.3)$$

where $\{\alpha_1, \dots, \alpha_{N+1}\}$ are different positive constants, $A = \max_{1 \leq s \leq N+1} \alpha_s$ and $\mathbf{c}_N = \{c_1, \dots, c_{N+1}\}$ satisfy the system

$$\sum_{s=1}^{N+1} c_s (-\alpha_s)^k = 1, \quad k = 0, \dots, N.$$

For example, if $\alpha_s = 1/2^s$ (extension 1) we have

$$\begin{aligned} \mathbf{c}_2 &= \{15, -54, 40\}, \mathbf{c}_4 = \{561/7, -10098/7, 7480, -95040/7, 52224/7\}, \\ \mathbf{c}_6 &= \{522665/1519, -5644782/217, 4181320/7, \\ &\quad -265636800/49, 145966080/7, -7114162176/217, 25490882560/1519\}; \end{aligned}$$

if $\alpha_s = 1/s$ (extension 2) then

$$\begin{aligned} \mathbf{c}_2 &= \{6, -32, 27\}, \mathbf{c}_4 = \{15, -640, 3645, -6144, 3125\}, \\ \mathbf{c}_6 &= \{28, -7168, 153090, -917504, 2187500, -2239488, 823543\}; \end{aligned}$$

if $\alpha_s = s$ (extension 3) then

$$\mathbf{c}_2 = \{6, -8, 3\}, \mathbf{c}_4 = \{15, -40, 45, -24, 5\}, \mathbf{c}_6 = \{28, -112, 210, -224, 140, -48, 7\}.$$

Obviously $\tilde{w} \in C^N([p - \frac{q-p}{A}, q + \frac{q-p}{A}])$ and

$$\|\tilde{w}\|_{W_\infty^N([p - \frac{q-p}{A}, q + \frac{q-p}{A}])} \leq c_1 \|w\|_{W_\infty^N([p, q])}.$$

Hence an extension of $g(\mathbf{x})$ with preserved smoothness is

$$\tilde{g}(\mathbf{x}) = \prod_{j=1}^n \tilde{w}(x_j)$$

and an approximate solution of (4.1) is given by

$$\begin{aligned} & \tilde{\mathcal{P}}_{M,h}(g)(\mathbf{x}, t) = \\ & \prod_{j=1}^n \frac{1}{\mathcal{D}^{1/2}} \sum_{hm_j \in I} \tilde{w}(hm_j) \left(\Phi_M \left(\frac{4t}{h^2 \mathcal{D}}, \frac{x_j - hm_j}{h\sqrt{\mathcal{D}}}, \frac{p - hm_j}{h\sqrt{\mathcal{D}}} \right) - \Phi_M \left(\frac{4t}{h^2 \mathcal{D}}, \frac{x_j - hm_j}{h\sqrt{\mathcal{D}}}, \frac{q - hm_j}{h\sqrt{\mathcal{D}}} \right) \right) \end{aligned} \quad (4.4)$$

with $I = (p - r\sqrt{\mathcal{D}}, q + r\sqrt{\mathcal{D}})$.

We provide results of some experiments which show accuracy and numerical convergence orders of the method. If we assume $[p, q] = [-1, 1]$ and $w(x) = e^{-x^2+ax}$ in (4.2), then problem (4.1) has the solution

$$u(\mathbf{x}, t) = \prod_{j=1}^n \frac{e^{\frac{a^2 t + ax_j - x_j^2}{4t+1}}}{2\sqrt{4t+1}} \left(\operatorname{erfc} \left(\frac{2(a-2)t + x_j - 1}{2\sqrt{t}\sqrt{4t+1}} \right) - \operatorname{erfc} \left(\frac{2(a+2)t + x_j + 1}{2\sqrt{t}\sqrt{4t+1}} \right) \right).$$

In Table 1 we compare the values of the exact solution and the approximate solution at some points in dimension $n = 1$. We choose the Hestenes extension corresponding to $\alpha_s = 1/s$. In Figure 1 we report on the absolute error for the solution of (4.1) at some grid points for space dimensions $n = 10^h$, $h = 1, \dots, 5$. We considered Hestenes extension with $\alpha_s = 1/2^s$. The approximations in Table 1 and Figure 1 have been computed on a uniform grid with step size $h = 1/80$ and $N = 6$. We assumed $\mathcal{D} = 4$ in order to have the saturation error comparable with the double precision rounding errors.

If g allows the representation (3.3), then, denoting by $\varepsilon_j^{(p)}$ the 1-dimensional error for each function $g_j^{(p)}$, the forms of the exact and the approximate solution obviously imply that the total error $\varepsilon_n = \mathcal{O}(\sum_{p=1}^P \sum_{j=1}^n \varepsilon_j^{(p)})$. Our numerical results confirm for the special choice of g that the n -dimensional error ε_n depends on the 1-dimensional error ε_1 like $\varepsilon_n = \mathcal{O}(n \varepsilon_1)$.

x	exact value	approximation	absolute error
-0.4	0.8612199065523	0.8612199065860	3.365E-011
-0.2	0.9367660745147	0.9367660745540	3.931E-011
0.0	0.9999999999999	1.0000000000044	4.465E-011
0.2	1.047614431487	1.047614431536	4.937E-011
0.4	1.077003231155	1.077003231208	5.322E-011
0.6	1.086497191179	1.086497191235	5.598E-011
0.8	1.075520922252	1.075520922309	5.749E-011
1.0	1.044650316417	1.044650316475	5.769E-011

Table 1: Exact, approximated values and absolute errors for the solution of (4.1) with $w(x) = e^{-x^2+ax}$ in (4.2), $a = 2.97109077126449$, and the Hestenes extension corresponding to $\alpha_s = 1/s$ using $\tilde{\mathcal{P}}_{3,0.0125}$, in $x \in \mathbb{R}$, $t = 1$.

In Tables 2 and 3 we show that formula (4.4) approximates the exact solution with the predicted approximate orders (2.5) in the space dimensions $n = 3, 10, 10^2, 10^3, 10^4, 10^5$. We assumed $w(x) = e^{(x+a)^2}$ which gives the exact solution of (4.1)

$$u(\mathbf{x}, t) = \prod_{j=1}^n \frac{e^{-\frac{(a+x_j)^2}{4t-1}}}{2\sqrt{4t-1}} \left(\operatorname{erfi} \left(\frac{4(a+1)t + x_j - 1}{2\sqrt{t}\sqrt{4t-1}} \right) - \operatorname{erfi} \left(\frac{4(a-1)t + x_j + 1}{2\sqrt{t}\sqrt{4t-1}} \right) \right).$$

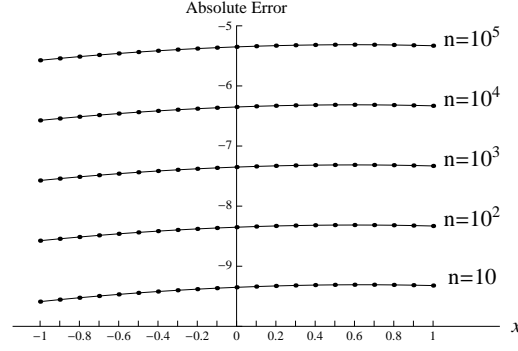


Figure 1: Absolute errors, using \log_{10} scale on the vertical axes, for the solution of (4.1) with $w(x) = e^{-x^2+ax}$ in (4.2), $a = 2.97109077126449$, and the Hestenes extension corresponding to $\alpha_s = 1/2^s$ using $\tilde{\mathcal{P}}_{3,0.0125}$, in $(x, 0, \dots, 0) \in \mathbb{R}^n$, $t = 1$, $x \in [-1, 1]$.

erfi denotes the imaginary error function defined as $\operatorname{erfi}(z) = -i \operatorname{erf}(iz)$. We choose $a = 0.575770212624068$, the extension $\tilde{w}(x) = w(x)$ in Table 2 and the Hestenes extension with $\alpha_s = 1/2^s$ in Table 3. For very high dimensional cases the second order formula fails, whereas the sixth order formula approximates with the predicted approximation rate. In all the cases the numerical results coincide with those if using other Hestenes extensions.

	h^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
$n = 3$	80	3.468E-03		4.231E-06		4.904E-09	
	160	8.655E-04	2.00	2.640E-07	4.00	7.633E-11	6.00
	320	2.162E-04	2.00	1.649E-08	4.00	1.141E-12	6.06
$n = 10$	80	1.154E-02		1.403E-05		1.624E-08	
	160	2.875E-03	2.00	8.753E-07	4.00	2.529E-10	6.00
	320	7.182E-04	2.00	5.468E-08	4.00	3.782E-12	6.06
$n = 100$	80	0.121E+00		1.400E-04		1.625E-07	
	160	2.908E-02	2.06	8.735E-06	4.00	1.670E-09	6.60
	320	7.194E-03	2.01	5.457E-07	4.00	2.006E-11	6.37

Table 2: Absolute errors and approximation rates for the solution of (4.1) with $w(x) = e^{(x+a)^2}$ in (4.2), $a = 0.575770212624068$, at the point $\mathbf{x} = (0.3, 0, \dots, 0)$, $t = 2$ using the approximation formula (4.4) and the extension $\tilde{w}(x) = w(x)$.

4.2 Nonhomogeneous problem

Here we provide results for the approximation of the solution of the problem

$$\frac{\partial u}{\partial t} - \Delta_{\mathbf{x}} u = f(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \mathbb{R}^n \times \mathbb{R}_+, \quad u(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \mathbb{R}^n \quad (4.5)$$

with $\operatorname{supp} f \subseteq [-1, 1]^n \times \mathbb{R}_+$.

	h^{-1}	$M = 2$		$M = 3$	
		error	rate	error	rate
$n = 1000$	80	1.395E-03		1.625E-06	
	160	8.727E-05	3.99	1.669E-08	6.60
	320	5.455E-06	3.99	2.007E-10	6.37
$n = 10000$	80	1.386E-02		1.617E-05	
	160	8.724E-04	3.99	1.669E-07	6.60
	320	5.455E-05	3.99	2.007E-09	6.37
$n = 100000$	80	0.130E+00		1.625E-04	
	160	8.690E-03	3.90	1.669E-06	6.60
	320	5.453E-04	3.99	2.007E-08	6.37

Table 3: Absolute errors and approximation rates for the solution of (4.1) with $w(x) = e^{(x+a)^2}$ in (4.2), $a = 0.575770212624068$, at the point $\mathbf{x} = (0.3, 0, \dots, 0)$, $t = 2$ using the approximation formula (4.4) and the Hestenes extension $\alpha_s = 1/2^s$.

Assuming (2.9), the approximate solution of (4.5) is

$$\begin{aligned} \tilde{\mathcal{H}}_{h,\tau}^{(M,M_0)}(f)(h\mathbf{k}, \tau\ell) &= \frac{\tau\ell\kappa\pi}{2\sqrt{\mathcal{D}_0}\mathcal{D}^n} \sum_{s=-S}^S \omega_s \sum_{i=-r_0\sqrt{\mathcal{D}_0}}^{T/\tau+r_0\sqrt{\mathcal{D}_0}} \eta_{2M_0} \left(\frac{\ell/(1 + e^{\pi \sinh(\kappa s)}) - i}{\sqrt{\mathcal{D}_0}} \right) \times \\ &\sum_{p=1}^P \beta_p \prod_{j=1}^n \sum_{|m_j| \leq 1/h+r\sqrt{\mathcal{D}}} f_j^{(p)}(hm_j, \tau i) \left(\Phi_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}}, P_{\mathbf{m}_j} \right) \right. \\ &\quad \left. - \Phi_M \left(\frac{4\tau\ell}{a_s h^2 \mathcal{D}}, \frac{k_j - m_j}{\sqrt{\mathcal{D}}} - \frac{2b_j\tau\ell}{a_s h \sqrt{\mathcal{D}}}, Q_{\mathbf{m}_j} \right) \right). \end{aligned}$$

First we demonstrate the effectiveness of the method on 1–dimensional examples, where an explicit solution can be obtained in a closed analytic form. We computed the solution of (4.5) with $f_i(x, t) = v(t)w_i(x)$, $\text{supp } w_i \subseteq [-1, 1]$, $i = 1, 2$, with $v(t) = t$, $w_1(x) = x e^x$ and $w_2(x) = e^x$.

We extend $w_i(x)$ outside $[-1, 1]$ by (4.3) and $v(t)$ outside \mathbb{R}_+ by

$$\tilde{v}(t) = \begin{cases} v(t), & t \geq 0 \\ \sum_{s=1}^{N+1} c_s v(-\alpha_s t), & t < 0 \end{cases}$$

where $\{c_s\}$ and $\{\alpha_s\}$ are defined in section 4.1.

In Table 4 we compare the exact value $\mathcal{H}_{[-1,1]}^{(0,0)} f_1$ and the approximate value $\tilde{\mathcal{H}}_{h,\tau}^{(3,3)} f_1$ at some points (x, t) of the grid. In numerical calculation we used the x –step size $h = 0.025$, the t –step size $\tau = 0.05$ and the Hestenes extension with $\alpha_s = s$, $T = 2$. The computational time on a 2 cpu Xeon Quad-Core processor with 2.4 Ghz is 0.26 seconds. If the dimension n is greater than 1, the approximation of the potential requires to compute $2SPn$ of one-dimensional operations and then the computational time scales linearly in the space dimension n . In Table 5 we report on the absolute errors and the approximation rates for $\mathcal{H}_{[-1,1]}^{(0,0)} f_2$. We used the approximation $\tilde{\mathcal{H}}_{h,\tau}^{(M,M)} f_2$ for $M =$

1, 2, 3, with the extension $\tilde{w} = w, \tilde{v} = v$ (top) and the Hestenes extension $\alpha_s = 1/s$ (bottom). Other parameters were $T = 1, \mathcal{D} = \mathcal{D}_0 = 4$, and $\kappa = 0.01, S = 611$ in the trapezoidal rule.

x	t	exact value	approximation	error
-0.2	2	0.241701111254	0.241701111067	0.187E-09
0.0	2	0.375668941931	0.375668941588	0.343E-09
0.2	2	0.523215078618	0.523215078096	0.522E-09
0.4	2	0.668323882248	0.668323881517	0.732E-09
0.6	2	0.786080733070	0.786080732090	0.980E-09
0.8	2	0.839219032083	0.839219030806	0.128E-08
1.0	2	0.773578882908	0.773578881325	0.158E-08
1.2	2	0.636739215551	0.636739214238	0.131E-08

Table 4: Exact, approximated values and absolute error for the solution of (4.5) with $f_1(x, t) = tx e^x$ in $[-1, 1]$, at the point (x, t) using $\tilde{\mathcal{H}}_{0.025, 0.05}^{(3,3)}$ and the Hestenes extension corresponding to $\alpha_s = s$.

h^{-1}	τ^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
20	20	0.928E-03		0.155E-05		0.129E-08	
40	40	0.232E-03	2.00	0.966E-07	4.00	0.201E-10	6.00
80	80	0.579E-04	2.00	0.604E-08	4.00	0.315E-12	5.99
160	160	0.145E-04	2.00	0.377E-09	4.00	0.477E-14	6.04

h^{-1}	τ^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
20	20	0.124E-02		0.154E-05		0.128E-08	
40	40	0.309E-03	1.99	0.965E-07	3.99	0.201E-10	5.99
80	80	0.773E-04	1.99	0.604E-08	3.99	0.310E-12	6.01
160	160	0.193E-04	2.00	0.377E-09	3.99	0.268E-13	3.53

Table 5: Absolute error and rate of convergence for $\mathcal{H}_{[-1,1]}^{(0,0)} f_2(0.2, 1)$ using $\tilde{\mathcal{H}}_{h,\tau}^{(3,3)}$ with the extension $\tilde{w} = w, \tilde{v} = v$ (top) and the Hestenes extension corresponding to $\alpha_s = 1/s$ (bottom).

The method is effective also if the dimension n is greater than 1, but we don't know any closed form analytic solution for right hand sides $f(\mathbf{x}, t)$ with nonvanishing values on the boundary $\partial[\mathbf{P}, \mathbf{Q}]$. Therefore we conclude this section with some results for right hand sides

$$f(\mathbf{x}, t) = \left(\frac{\partial}{\partial t} - \Delta_{\mathbf{x}} \right) \prod_{j=1}^n w(x_j) v(t) = \sum_{p=1}^n \prod_{j=1}^n f_j^{(p)}(x_j, t), \quad \mathbf{x} = (x_1, \dots, x_n) \in [-1, 1]^n; \quad (4.6)$$

$$f_j^{(p)}(x, t) = w(x) \quad \text{if } j \neq p, \quad f_j^{(j)}(x, t) = \frac{1}{n} v'(t) w(x) - v(t) w''(x)$$

where $\text{supp } w \subseteq [-1, 1]$ and $\text{supp } v \subseteq \mathbb{R}_+$. If $w(\pm 1) = w'(\pm 1) = 0$ and $v(0) = 0$, then the solution of (4.5) is $u(\mathbf{x}, t) = \prod_{j=1}^n w(x_j) v(t)$.

Figure 2 shows absolute errors at some grid points for the solution of (4.5) in dimensions $n = 10, 20, 40, 60, 80, 100$. The approximations have been computed using $\tilde{\mathcal{H}}_{h,\tau}^{(3,3)}$ on a uniform grid with x -step size $h = 1/160$ and t -step size $\tau = 1/160$, with $M = M_0 = 3, T = 2$, the Hestenes

extension corresponding to $\alpha_s = 1/2^s$, $w(x) = e^x(x^2 - 1)^2$ and $v(t) = t$. The parameters were $\mathcal{D} = \mathcal{D}_0 = 4$, and $\kappa = 0.02$, $S = 305$ in the trapezoidal rule.

If f allows the representation (2.9), then the n - dimensional error $\varepsilon_n = \mathcal{O}\left(\sum_{p=1}^P \sum_{j=1}^n \varepsilon_j^{(p)}\right)$, where $\varepsilon_j^{(p)}$

denotes the 1- dimensional error for each function $f_j^{(p)}$. Our numerical experiments confirm that, for the special choice of f in (4.6) with the separation rank $P = n$, the total error $\varepsilon_n = \mathcal{O}(n^2\varepsilon_1)$.

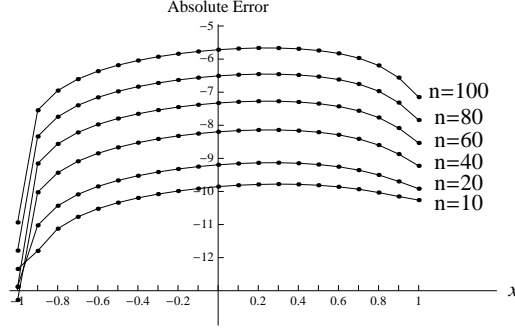


Figure 2: Absolute errors, using \log_{10} scale on the vertical axes, for the solution of (4.5) with $f(\mathbf{x}, t)$ in (4.6) where $w(x) = e^x(x^2 - 1)^2$ and $v(t) = t$, at the point $(x, 0.1, \dots, 0.1, 2) \in \mathbb{R}^n \times \mathbb{R}_+$ using $\tilde{\mathcal{H}}_{h,\tau}^{(3,3)}$ with $h = \tau = 1/160$ and the Hestenes extension corresponding to $\alpha_s = 1/2^s$.

In Table 6 we report on the absolute errors and the approximation rates in the space dimensions $n = 3, 10, 100, 200$ for the solution of (4.5). We assumed $w(x) = e^x(x^2 - 1)^2$ and $v(t) = 1 - e^{-t}$ in (4.6). The approximations have been computed by $\tilde{\mathcal{H}}_{h,\tau}^{(M,M)}$ for $M = 1, 2, 3$, $T = 4$ and the Hestenes extension with $\alpha_s = 1/s$. The results show that, for high dimensions, the second order formula fails whereas the fourth and sixth order formulas approximate with the predicted approximation rates.

	h^{-1}	τ^{-1}	$M = 1$		$M = 2$		$M = 3$	
			error	rate	error	rate	error	rate
$n = 3$	80	40	0.799E-03		0.383E-05		0.175E-08	
	160	80	0.214E-03	1.90	0.244E-06	3.97	0.277E-10	5.98
	320	160	0.553E-04	1.95	0.154E-07	3.98	0.485E-12	5.83
	640	320	0.137E-04	2.01	0.955E-09	4.00	0.933E-14	5.70
$n = 10$	80	40	0.831E-02		0.148E-05		0.335E-08	
	160	80	0.208E-02	1.99	0.917E-07	4.00	0.523E-10	6.00
	320	160	0.521E-03	1.99	0.572E-08	4.00	0.809E-12	6.01
	640	320	0.131E-03	1.99	0.337E-09	4.08	0.133E-14	9.24
$n = 100$	80	40			0.239E-01		0.455E-04	
	160	80			0.149E-02	4.00	0.710E-06	6.00
	320	160			0.931E-04	4.00	0.110E-07	6.01
	640	320			0.579E-05	4.00	0.196E-10	9.13
$n = 200$	80	40					0.269E+00	
	160	80			0.891E+01		0.420E-02	6.00
	320	160			0.556E+00	4.00	0.651E-04	6.01
	640	320			0.347E-01	4.00	0.122E-06	9.06

Table 6: Absolute errors and approximation rates for the solution of (4.5) with $f(\mathbf{x}, t)$ in (4.6) where $w(x) = e^x(x^2 - 1)^2$ and $v(t) = 1 - e^{-t}$, at the point $\mathbf{x} = (-0.2, 0.1, \dots, 0.1)$; $t = 4$ using $\tilde{\mathcal{H}}_{h,\tau}^{(M,M)}$ and the Hestenes extension corresponding to $\alpha_s = 1/s \dots$

References

- [1] M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions*. Dover. Publ., New York, 1968.
- [2] G. Beylkin, R. Cramer, G. Fann, and R. J. Harrison. Multiresolution separated representations of singular and weakly singular operators. *Appl. Comput. Harmon. Anal.*, 23(2):235–253, 2007.
- [3] G. Beylkin, G. Fann, R. J. Harrison, C. Kurcz, and L. Monzón. Multiresolution representation of operators with boundary conditions on simple domains. *Appl. Comput. Harmon. Anal.*, 33(1):109–139, 2012.
- [4] G. Beylkin, J. Garcke, and M. J. Mohlenkamp. Multivariate regression and machine learning with sums of separable functions. *SIAM J. Sci. Comput.*, 31(3):1840–1857, 2009.
- [5] G. Beylkin, C. Kurcz, and L. Monzón. Fast convolution with the free space Helmholtz Green’s function. *J. Comput. Phys.*, 228(8):2770–2791, 2009.
- [6] G. Beylkin and M. J. Mohlenkamp. Numerical operator calculus in higher dimensions. *Proc. Natl. Acad. Sci. USA*, 99(16):10246–10251, 2002.
- [7] G. Beylkin and M. J. Mohlenkamp. Algorithms for numerical analysis in high dimensions. *SIAM J. Sci. Comput.*, 26(6):2133–2159, 2005.

- [8] L. C. Evans. *Partial differential equations*, volume 19 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, second edition, 2010.
- [9] I. P. Gavrilyuk, W. Hackbusch, and B. N. Khoromskij. Hierarchical tensor-product approximation to the inverse and related operators for high-dimensional elliptic problems. *Computing*, 74(2):131–157, 2005.
- [10] L. Grasedyck, D. Kressner, and C. Tobler. A literature survey of low-rank tensor approximation techniques. *GAMM-Mitt.*, 36(1):53–78, 2013.
- [11] W. Hackbusch. Efficient convolution with the Newton potential in d dimensions. *Numer. Math.*, 110(4):449–489, 2008.
- [12] W. Hackbusch. *Tensor Spaces and Numerical Tensor Calculus*, volume 42 of *Springer Series in Computational Mathematics*. Springer-Verlag Berlin Heidelberg, 2012.
- [13] W. Hackbusch and B. N. Khoromskij. Tensor-product approximation to multidimensional integral operators and Green’s functions. *SIAM J. Matrix Anal. Appl.*, 30(3):1233–1253, 2008.
- [14] M. R. Hestenes. Extension of the range of a differentiable function. *Duke Math. J.*, 8:183–192, 1941.
- [15] B. N. Khoromskij. Fast and accurate tensor approximation of a multivariate convolution with linear scaling in dimension. *J. Comput. Appl. Math.*, 234(11):3122–3139, 2010.
- [16] F. Lanzara, V. Maz’ya, and G. Schmidt. On the fast computation of high dimensional volume potentials. *Math. Comp.*, 80(274):887–904, 2011.
- [17] F. Lanzara, V. Maz’ya, and G. Schmidt. Fast cubature of volume potentials over rectangular domains by approximate approximations. *Appl. Comput. Harmon. Anal.*, 36(1):167–182, 2014.
- [18] F. Lanzara, V. G. Maz’ya, and G. Schmidt. Accurate cubature of volume potentials over high-dimensional half-spaces. *J. Math. Sci. (N. Y.)*, 173(6):683–700, 2011.
- [19] F. Lanzara and G. Schmidt. On the computation of high-dimensional potentials of advection-diffusion operators. *Mathematika*, 61:309–327, 2015.
- [20] V. Maz’ya. *Sobolev spaces with applications to elliptic partial differential equations*, volume 342 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer, Heidelberg, augmented edition, 2011.
- [21] V. Maz’ya and G. Schmidt. *Approximate approximations*, volume 141 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2007.
- [22] H. Takahasi and M. Mori. Double exponential formulas for numerical integration. *Publ. Res. Inst. Math. Sci.*, 9:721–741, 1973/74.
- [23] J. Waldvogel. Towards a general error theory of the trapezoidal rule. In *Approximation and computation*, volume 42 of *Springer Optim. Appl.*, pages 267–282. Springer, New York, 2011.