

Approximation of solutions to multidimensional parabolic equations by Approximate Approximations

F. Lanzara¹ , V. Maz'ya² , G. Schmidt³

¹ *Department of Mathematics, Sapienza University of Rome,
Piazzale Aldo Moro 2, 00185 Rome, Italy
lanzara@mat.uniroma1.it*

² *Department of Mathematics, University of Linköping,
581 83 Linköping, Sweden;
Department of Mathematical Sciences, M&O Building,
University of Liverpool, Liverpool L69 3BX, UK;
vlmaz@mai.liu.se*

³ *Weierstrass Institute for Applied Analysis and Stochastics,
Mohrenstr. 39, 10117 Berlin, Germany
schmidt@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, make 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 6 up to dimension 10^7 .

AMS subject classifications. 65D32, 41A30, 41A63.

Keywords: Higher dimensions, separated representations, parabolic equation, multi-dimensional convolution.

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, 4, 5, 9, 10, 11, 13] and the references therein) to some class of multidimensional integral operators. Some algorithms approximate the operator kernel via a separated representation given by a linear combination of exponentials or Gaussians, which yields a form with elements given by one-dimensional sums. As a result, efficient fast algorithms in dimensions 2 and 3 are obtained, which permit further generalizations to

dimensions greater than 3. 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. The difficulty is the necessity to find accurate separated representations of the integral operator acting on piecewise polynomials, especially for higher order approximations. The convergence orders 2 and 3 were confirmed by numerical experiments in dimension 3.

A new method of an arbitrary high order and high accuracy, which does not approximate or modify the kernel of the integral operator, was recently introduced in [14] and [15] for the cubature of high dimensional Newton potential over the full space and over half spaces. The density is approximated by the 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. For the potential of advection-diffusion over hyper-rectangular domains, the corresponding new method was introduced in [16] and, more generally, in [17].

In this paper we propose a fast method in the framework of approximate approximations for the n -dimensional time dependent problem

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

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]

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

where

$$\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} g(\mathbf{x}, t) = \frac{e^{-ct}}{(4\pi t)^{n/2}} \int_{[\mathbf{P}, \mathbf{Q}]} e^{-|\mathbf{x} - \mathbf{y} - 2\mathbf{b}t|^2/(4t)} g(\mathbf{y}) d\mathbf{y}, \tag{1.2}$$

$$\begin{aligned} \mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f(\mathbf{x}, t) &= \int_0^t \frac{e^{-cs} ds}{(4\pi s)^{n/2}} \int_{[\mathbf{P}, \mathbf{Q}]} e^{-|\mathbf{x} - \mathbf{y} - 2\mathbf{b}s|^2/(4s)} f(\mathbf{y}, t - s) d\mathbf{y} \\ &= \int_0^t (\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f(\cdot, s))(\mathbf{x}, t - s) ds. \end{aligned} \tag{1.3}$$

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 that is it is represented as product of functions depending only on one of the space variables. Then a separated representation of the initial condition g provides a separated representation of the potential. Moreover, $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})} f$ is expressed as a one-dimensional integral with separated integrand. This construction, combined with an accurate quadrature rule as suggested in [13] and a separated representation of the density f , provides a separated representation of the integral operator (1.3). Only one-dimensional operations are used. We derive formulas of an

arbitrary high order, fast and accurate also in very high dimensions. The accuracy of the method and the convergence orders 2, 4 and 6 are confirmed by numerical experiments up to dimension $n = 10^7$.

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 very high.

2 Description of the method

The functions f and g in (1.1) are approximated by quasi-interpolant on the rectangular grids $\{(h\mathbf{m}, \tau i)\}$ and $\{h\mathbf{m}\}$, respectively,

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

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

where τ, 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. ([18, 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*

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

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

We construct an approximation of the solution of (1.1) if we approximate f and g such that the integrals $\mathcal{P}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})}$ and $\mathcal{H}_{[\mathbf{P}, \mathbf{Q}]}^{(c, \mathbf{b})}$ applied to it can be computed, analytically or at least efficiently. This can be done if we approximate g in $[\mathbf{P}, \mathbf{Q}]$ and f in $[\mathbf{P}, \mathbf{Q}] \times \mathbb{R}_+$ by means of the approximate 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 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 ([12], see also [19, 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

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

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 $I_j = (P_j - rh\sqrt{\mathcal{D}}, Q_j + rh\sqrt{\mathcal{D}})$. Then the sum

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

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

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

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

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

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*

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

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 $\{(h\mathbf{k}, \tau\ell)\}$,

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

In the following we denote the two terms on the right by Σ_1 and Σ_2 .

It can be easily seen that from (1.2)

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

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])

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

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, they can be represented as sum of products of univariate functions

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

Then the first term in (2.7) 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 on the right of (2.7) involves additionally an integration, which must be approximated by an efficient quadrature. The integral

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

cannot be taken analytically. Therefore we use a quadrature based on the classical trapezoidal rule. It is known that it is exponentially converging for rapidly decaying smooth functions on the real line (see [21, 20]). 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 [20], 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 quadrature with 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 the second term Σ_2 on the right of (2.7) 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 an 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. We assume that $\eta(\mathbf{x})$ is the product of univariate basis functions of the form Gaussians times special polynomials

$$\eta(\mathbf{x}) = \prod_{j=1}^n \eta_{2M}(x_j); \quad \eta_{2M}(x_j) = \frac{(-1)^{M-1}}{2^{2M-1} \sqrt{\pi} (M-1)!} \frac{H_{2M-1}(x_j) e^{-x_j^2}}{x_j} \quad (2.13)$$

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. [18, p.56]).

3 High order cubature formulas

To get formulas similar to (2.12) for higher order approximations, we approximate the density with quasi-interpolants based on (2.13). We start with the following

Theorem 3.1. *Let $M \geq 1$. The integral (1.2) applied to the generating function $\prod_{j=1}^n \eta_{2M}(x_j)$ in (2.13) can be written as*

$$(\mathcal{P}_{[P,Q]}^{(c,b)}(\prod_{j=1}^n \eta_{2M}(\cdot)))(\mathbf{x}, t) = e^{-ct} \prod_{j=1}^n (\Phi_M(4t, x_j - 2b_j t, P_j) - \Phi_M(4t, x_j - 2b_j t, Q_j)) \quad (3.1)$$

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 (1.2) 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 ([18, 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 [16, 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 (3.1) 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

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

for the generating function η defined in (2.13). 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

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

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

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

where now

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

Similarly, we specify the approximation

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

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

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

where, in view of (2.13) 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

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

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)

$$u_{h,\tau}(h\mathbf{k}, \tau\ell) \approx \frac{e^{-c\tau\ell}}{\mathcal{D}^{n/2}} \sum_{p=1}^P \alpha_p \prod_{j=1}^n S_j^{(p)}(k_j, \tau\ell) \\ + \frac{\tau\ell\kappa\pi}{2\sqrt{\mathcal{D}_0}\mathcal{D}^n} \sum_{s=-S}^S \omega_s e^{-c\tau\ell/a_s} \sum_{\tau i \in \tilde{\Omega}_{r_0\tau}} \eta_{2M_0} \left(\frac{\ell/(1 + e^{\pi \sinh(\kappa s)}) - i}{\sqrt{\mathcal{D}_0}} \right) \sum_{p=1}^P \beta_p \prod_{j=1}^n T_j^{(p)}(k_j, \tau\ell, \tau i, a_s),$$

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

Remark 3.1. Consider the initial value problem for the parabolic equation

$$\frac{\partial u}{\partial t} - A \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} u + 2\mathbf{b} \cdot \nabla_{\mathbf{x}} u + c u = f(\mathbf{x}, t) \quad \text{in } \mathbb{R}^n \times \mathbb{R}_+ \quad (3.2)$$

$$u(\mathbf{x}, 0) = g(\mathbf{x}) \quad \text{on } \mathbb{R}^n. \quad (3.3)$$

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 (3.2), (3.3) reduces to the initial value problem

$$\frac{\partial U}{\partial t} - \Delta_{\boldsymbol{\xi}} U + 2\boldsymbol{\beta} \cdot \nabla_{\boldsymbol{\xi}} U + c U = F(\boldsymbol{\xi}, t) \quad \text{in } \mathbb{R}^n \times \mathbb{R}_+ \quad (3.4)$$

$$U(\boldsymbol{\xi}, 0) = G(\boldsymbol{\xi}) \quad \text{on } \mathbb{R}^n. \quad (3.5)$$

The solution of (3.4), (3.5) can be represented as

$$U(\boldsymbol{\xi}, t) = \mathcal{P}^{(c, \boldsymbol{\beta})}(G(\cdot))(\boldsymbol{\xi}, t) + \int_0^t (\mathcal{P}^{(c, \boldsymbol{\beta})} F(\cdot, s))(\boldsymbol{\xi}, t - s) ds \quad (3.6)$$

where

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

An approximate solution of (3.4), (3.5) can be obtained by using the generating function [18, 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. [18, 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 (3.6) 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 (3.2)

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

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

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

4 Numerical Results

4.1 Initial-value problem

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

$$\frac{\partial u}{\partial t} - \Delta_{\mathbf{x}} u = 0, \quad (\mathbf{x}, t) \in \mathbb{R}^n \times \mathbb{R}_+; \quad u(\mathbf{x}, 0) = g(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n \quad (4.7)$$

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

$$g(\mathbf{x}) = \prod_{j=1}^n w(x_j), \quad \mathbf{x} = (x_1, \dots, x_n) \in [p, q]^n \quad (4.8)$$

and $w \in C^N([p, q])$.

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

$$\tilde{w}(x) = \begin{cases} \sum_{s=1}^{N+1} c_s w(-\alpha_s(x - q) + q), & q < x \leq q + \frac{q-p}{A} \\ w(x), & p \leq x \leq q \\ \sum_{s=1}^{N+1} c_s w(-\alpha_s(x - p) + p), & p - \frac{q-p}{A} \leq x < p \end{cases} \quad (4.9)$$

where $\{a_1, \dots, a_{N+1}\}$ 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 (4.7) is given by

$$\begin{aligned} \tilde{\mathcal{P}}_{M,h}(g)(\mathbf{x}, t) = \\ \prod_{j=1}^n \frac{1}{\mathcal{D}^{1/2}} \sum_{hm_j \in I_j} \tilde{w}(hm_j) \left(\Phi_M \left(\frac{4t}{h^2 \mathcal{D}}, \frac{x_j - hm_j}{h\sqrt{\mathcal{D}}}, \frac{p - hm_j}{h\sqrt{\mathcal{D}}} \right) - \Phi_M \left(\frac{4t}{h^2 \mathcal{D}}, \frac{x_j - hm_j}{h\sqrt{\mathcal{D}}}, \frac{q - hm_j}{h\sqrt{\mathcal{D}}} \right) \right). \end{aligned} \quad (4.10)$$

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 (4.8), then problem (4.7) has exact value

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

In Table 1 we compare the values of the exact solution and the approximate solution at some points in dimensions $n = 3, 10, 100$. We choose the Hestenes extension corresponding to $\alpha_s = 1/s$.

Table 2 shows that the method is effective also for higher space dimensions. We report on exact values and absolute errors for the solution of (4.7) at some grid points for space dimensions $n = 10^3, 10^4, 10^5$. We considered Hestenes extension with $\alpha_s = 1/2^s$. The approximations in Table 1 and 2 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.

In Tables 3, 4 and 5 we show that formula (4.10) approximates the exact solution with the predicted approximate orders (2.5) in the space dimensions $n = 3, 10, 10^2, 10^3, 10^4, 10^5$. In Table 3 we assumed $w(x) = e^{-x^2}$ and the Hestenes extension $\alpha_s = s$; in Tables 4 and 5 we assumed $w(x) = e^{(x+a)^2}$ which gives the exact solution of (4.7)

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

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 4 and the Hestenes extension with $\alpha_s = 1/2^s$ in Table 5. 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.

4.2 Nonhomogeneous problem

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

$$\frac{\partial u}{\partial t} - \Delta_{\mathbf{x}} u = f(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \mathbb{R}^n \times \mathbb{R}_+, \quad u(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \mathbb{R}^n \quad (4.11)$$

dimension	x	exact value	approximation	absolute error
$n = 3$	-0.4	0.86121990655	0.86121990666	1.1056E-10
	-0.2	0.93676607451	0.93676607463	1.2297E-10
	0.0	0.99999999999	1.00000000013	1.3395E-10
	0.2	1.04761443148	1.04761443163	1.4293E-10
	0.4	1.07700323115	1.07700323130	1.4940E-10
	0.6	1.08649719117	1.08649719133	1.5301E-10
	0.8	1.07552092225	1.07552092240	1.5354E-10
	1.0	1.04465031641	1.04465031656	1.5098E-10
$n = 10$	-0.4	0.86121990655	0.86121990693	3.7976E-10
	-0.2	0.93676607451	0.93676607493	4.1578E-10
	0.0	0.99999999999	1.00000000044	4.4652E-10
	0.2	1.04761443148	1.04761443195	4.7038E-10
	0.4	1.07700323115	1.07700323164	4.8604E-10
	0.6	1.08649719117	1.08649719167	4.9261E-10
	0.8	1.07552092225	1.07552092274	4.8971E-10
	1.0	1.04465031641	1.04465031689	4.7751E-10
$n = 100$	-0.4	0.86121990655	0.86121991039	3.8407E-09
	-0.2	0.93676607451	0.93676607869	4.1804E-09
	0.0	0.99999999999	1.00000000446	4.4652E-09
	0.2	1.04761443148	1.04761443616	4.6804E-09
	0.4	1.07700323115	1.07700323596	4.8142E-09
	0.6	1.08649719117	1.08649719603	4.8589E-09
	0.8	1.07552092225	1.07552092706	4.8119E-09
	1.0	1.04465031641	1.04465032109	4.6757E-09

Table 1: Exact, approximated values and absolute errors for the solution of (4.7) with $w(x) = e^{-x^2+ax}$ in (4.8), $a = 2.97109077126449$, and the Hestenes extension corresponding to $\alpha_s = 1/s$ using $\tilde{\mathcal{P}}_{6,0.0125}$, in $(x, 0, \dots, 0) \in \mathbb{R}^n$, $t = 1$.

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

Assuming (2.9), the approximate solution of (4.11) is

$$\begin{aligned} \tilde{\mathcal{H}}_{h,\tau}^{(M,M_0)}(f)(h\mathbf{k}, \tau\ell) &= \frac{\tau\ell\kappa\pi}{2\sqrt{\mathcal{D}_0}\mathcal{D}^n} \sum_{s=-S}^S \omega_s \sum_{\tau=r_0\sqrt{\mathcal{D}_0}}^{T/\tau+r_0\sqrt{\mathcal{D}_0}} \eta_{2M_0} \left(\frac{\ell/(1 + e^{\pi \sinh(\kappa s)}) - i}{\sqrt{\mathcal{D}_0}} \right) \\ &\times \sum_{p=1}^P \beta_p \prod_{j=1}^n \sum_{|m_j| \leq 1/h+r\sqrt{\mathcal{D}}} f_j^{(p)}(hm_j, \tau i) \times \left(\phi_{P_{m_j}}^{(0)} \left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{a_s h^2 \mathcal{D}} \right) - \phi_{Q_{m_j}}^{(0)} \left(\frac{k_j - m_j}{\sqrt{\mathcal{D}}}, \frac{\tau\ell}{a_s h^2 \mathcal{D}} \right) \right). \end{aligned}$$

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 (4.11) 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 $w_2(x) = e^x$.

n	1000		10000		100000	
x	exact value	error	exact value	error	exact value	error
-0.4	0.861219	3.8451E-08	0.861219	3.8455E-07	0.861219	3.8455E-06
-0.2	0.936766	4.1826E-08	0.936766	4.1829E-07	0.936766	4.1829E-06
0.0	0.999999	4.4652E-08	0.999999	4.4652E-07	0.999999	4.4652E-06
0.2	1.047614	4.6781E-08	1.047614	4.6779E-07	1.047614	4.6779E-06
0.4	1.077003	4.8096E-08	1.077003	4.8091E-07	1.077003	4.8091E-06
0.6	1.086497	4.8522E-08	1.086497	4.8515E-07	1.086497	4.8515E-06
0.8	1.075520	4.8034E-08	1.075520	4.8026E-07	1.075520	4.8025E-06
1.0	1.044650	4.6657E-08	1.044650	4.6647E-07	1.044650	4.6646E-06

Table 2: Exact values and absolute errors for the solution of (4.7) with $w(x) = e^{-x^2+ax}$ in (4.8), $a = 2.97109077126449$, at $(x, 0, \dots, 0) \in \mathbb{R}^n$, $t = 1$, using $\tilde{\mathcal{P}}_{6,0.0125}$ and the Hestenes extension corresponding to $\alpha_s = 1/s$.

We extend $w_i(x)$ outside $[-1, 1]$ by (4.9) 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 6 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 Tables 7 and 8 we report on the absolute errors and the approximation rates for $\mathcal{H}_{[-1,1]}^{(0,0)} f_2$. We used the approximation $\tilde{H}_{h,\tau}^{(M,M)} f_2$ for $M = 1, 2, 3$, with $\tilde{w} = w$, $\tilde{v} = v$ (Table 7) and the Hestenes extension $\alpha_s = 1/s$ (Table 8), $T = 1$. Other parameters were $\mathcal{D} = \mathcal{D}_0 = 4$, and $\kappa = 0.01$, $S = 611$ in the trapezoidal rule.

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

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

$$f_j^{(p)}(x, t) = w(x) \quad \text{if } j \neq p, \quad f_j^{(j)}(x, t) = \frac{1}{n}v'(t)w(x) - v(t)w''(x) \quad (4.12)$$

where $\text{supp } w \subseteq [-1, 1]$ and $\text{supp } v \subseteq \mathbb{R}_+$. If $w(\pm 1) = w_x(\pm 1) = 0$ and $v(0) = 0$, then the solution of (4.11) is $u(\mathbf{x}, t) = \prod_{j=1}^n w(x_j)v(t)$.

	h^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
$n = 3$	10	0.466E-01		0.127E-02		0.351E-04	
	20	0.120E-01	1.95	0.828E-04	3.93	0.635E-06	5.79
	40	0.304E-02	1.98	0.524E-05	3.98	0.100E-07	5.98
	80	0.761E-03	1.99	0.328E-06	3.99	0.157E-09	5.99
	160	0.190E-03	1.99	0.205E-07	3.99	0.246E-11	5.99
	320	0.476E-04	1.99	0.128E-08	3.99	0.386E-13	5.99
$n = 10$	10	0.112E+00		0.325E-02		0.928E-04	
	20	0.303E-01	1.88	0.213E-03	3.93	0.163E-05	5.82
	40	0.774E-02	1.97	0.134E-04	3.98	0.259E-07	5.98
	80	0.194E-02	1.99	0.843E-06	3.99	0.406E-09	5.99
	160	0.487E-03	1.99	0.527E-07	3.99	0.635E-11	5.99
	320	0.122E-03	1.99	0.330E-08	3.99	0.989E-13	6.00
$n = 100$	10	0.177E-01		0.100E-02		0.295E-04	
	20	0.780E-02	1.18	0.668E-04	3.90	0.513E-06	5.84
	40	0.231E-02	1.75	0.423E-05	3.98	0.814E-08	5.97
	80	0.602E-03	1.93	0.265E-06	3.99	0.128E-09	5.99
	160	0.152E-03	1.98	0.166E-07	3.99	0.200E-11	5.99
	320	0.382E-04	1.99	0.104E-08	3.99	0.311E-13	6.00

Table 3: Absolute errors and approximation rates for the solution of (4.7) with $w(x) = e^{-x^2}$ in (4.8), at the point $\mathbf{x} = (0.1, 0, \dots, 0)$, $t = 0.02$ using the approximation formula (4.10) and the Hestenes extension with $\alpha_s = s$.

In Table 9 we compare the values of exact and approximate solution of (4.11) at some points, in dimensions $n = 3, 10, 100, 1000$, if $w(x) = e^x(x^2 - 1)^2$ and $v(t) = t$. Table 10 shows that the algorithm is successful also for much higher space dimensions. The approximations have been computed using $\tilde{\mathcal{H}}_{0.0125, 0.0125}^{(3,3)}$ on a uniform grid with x -step size $h = 0.025$ and t -step size $\tau = 0.025$, with $M = M_0 = 3$, $T = 2$ and the Hestenes extension corresponding to $\alpha_s = 1/2^s$. The parameters were $\mathcal{D} = \mathcal{D}_0 = 4$, and $\kappa = 0.02$, $S = 305$ in the trapezoidal rule.

In Table 11 we report on the absolute errors and the approximation rates in the space dimensions $n = 3, 10^i$, $i = 1, \dots, 7$ for the solution of (4.11). We assumed $w(x) = \cos^2(\pi x/2)$ and $v(t) = 1 - e^{-t}$ in (4.12). 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 very high dimensions, the second order formula fails whereas the fourth and sixth order formulas approximate with the predicted approximation rates and the error scales linearly in the space dimension.

References

- [1] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, Dover Publ., New York, 1968.
- [2] G. Beylkin, R. Cramer, G. Fann, R. J. Harrison, Multiresolution separated representations of singular and weakly singular operators, Appl. Comput. Harmon. Anal. 23 (2007), 235–

	h^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
$n = 3$	10	0.259E+00		2.002E-02		1.594E-03	
	20	5.751E-02	2.17	1.121E-03	4.15	2.111E-05	6.23
	40	1.397E-02	2.04	6.818E-05	4.03	3.170E-07	6.05
	80	3.468E-03	2.01	4.231E-06	4.01	4.904E-09	6.01
	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
$n = 10$	10	1.020E+00		6.488E-02		5.292E-03	
	20	0.199E+00	2.35	3.713E-03	4.12	6.996E-05	6.24
	40	4.688E-02	2.08	2.260E-04	4.03	1.050E-06	6.05
	80	1.154E-02	2.02	1.403E-05	4.00	1.624E-08	6.01
	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
$n = 100$	10			0.490E+00		4.192E-02	
	20	5.254E+00		3.646E-02	3.75	6.569E-04	5.99
	40	0.581E+00	3.17	2.253E-03	4.01	1.031E-05	5.99
	80	0.121E+00	2.25	1.400E-04	4.00	1.625E-07	5.98
	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 4: Absolute errors and approximation rates for the solution of (4.7) with $w(x) = e^{(x+a)^2}$ in (4.8), $a = 0.575770212624068$, at the point $\mathbf{x} = (0.3, 0, \dots, 0)$, $t = 2$ using the approximation formula (4.10) and the extension $\tilde{w}(x) = w(x)$.

253.

- [3] G. Beylkin, G. Fann, R.J. Harrison, C. Kurcz, L. Monzón, Multiresolution representation of operators with boundary conditions on simple domains, *Appl. Comput. Harmon. Anal.* 33 (2012), 109–139.
- [4] G. Beylkin, C. Kurcz, L. Monzón, Fast convolution with the free space Helmholtz Greens function, *Journal of Computational Physics*, 228 (2009), 2770–2791.
- [5] I. Gavriluk, W. Hackbusch and B. N. Khoromskij, Hierarchical tensor-product approximation to the inverse and related operators for high-dimensional elliptic problems, *Computing*, 74 (2005), 131–157.
- [6] G. Beylkin, M.J. Mohlenkamp, Numerical operator calculus in higher dimensions, *Proc. Natl. Acad. Sci. USA*, 99 (2002), 10246–10251.
- [7] G. Beylkin, M.J. Mohlenkamp, Algorithms for numerical analysis in high dimensions, *SIAM J. Sci. Comput.* 26 (2005), 2133–2159.
- [8] L. C. Evans, *Partial Differential Equations*, v.19, AMS, 2010.
- [9] W. Hackbusch, Efficient convolution with the Newton potential in d dimensions, *Numer. Math.*, 110 (2008), 449–489.

	h^{-1}	$M = 2$		$M = 3$	
		error	rate	error	rate
$n = 1000$	20	0.300E+00		6.586E-03	
	40	2.207E-02	3.76	1.031E-04	5.99
	80	1.395E-03	3.98	1.625E-06	5.98
	160	8.727E-05	3.99	1.669E-08	6.60
	320	5.455E-06	3.99	2.007E-10	6.37
$n = 10000$	20	0.990E+00		6.781E-02	
	40	0.200E+00	2.30	1.031E-03	6.03
	80	1.386E-02	3.85	1.617E-05	5.98
	160	8.724E-04	3.99	1.669E-07	6.60
	320	5.455E-05	3.99	2.007E-09	6.37
$n = 100000$	20	1.021E+00		0.920E+00	
	40	0.906E+00	0.17	1.036E-02	6.47
	80	0.130E+00	2.79	1.625E-04	5.99
	160	8.690E-03	3.90	1.669E-06	6.60
	320	5.453E-04	3.99	2.007E-08	6.37

Table 5: Absolute errors and approximation rates for the solution of (4.7) with $w(x) = e^{(x+a)^2}$ in (4.8), $a = 0.575770212624068$, at the point $\mathbf{x} = (0.3, 0, \dots, 0)$, $t = 2$ using the approximation formula (4.10) and the Hestenes extension $\alpha_s = 1/2^s$.

- [10] W. Hackbusch and B. N. Khoromskij, Tensor-product approximation to operators and functions in high dimensions, *J. Complexity*, 23 (2007), 4–6.
- [11] W. Hackbusch and B. N. Khoromskij, Tensor-product approximation to multidimensional integral operators and Green’s functions, *SIAM J. Matrix Anal. Appl.*, 30 (2008), 1233–1253.
- [12] M. R. Hestenes, Extension of the range of differentiable functions. *Duke Math. J.* 8 (1941), 183–192.
- [13] B. N. Khoromskij, Fast and accurate tensor approximation of a multivariate convolution with linear scaling in dimension, *J. Comput. Appl. Math.*, 234 (2010) 3122–3139.
- [14] F. Lanzara, V. Maz’ya and G. Schmidt, On the fast computation of high dimensional volume potentials, *Math. Comput.*, 80 (2011), 887-904.
- [15] F. Lanzara, V. Maz’ya and G. Schmidt, Accuracy cubature of volume potentials over high-dimensional half-spaces, *J. Math. Sciences*, 173 (2011), 683–700.
- [16] F. Lanzara, V. Maz’ya and G. Schmidt, Fast cubature of volume potentials over rectangular domains by approximate approximations, *Appl. Comput. Harmon. Anal.* 36 (2014), 167–182.
- [17] F. Lanzara, V. Maz’ya and G. Schmidt, On the computation of high-dimensional potentials of advection- diffusion operators, to appear.

x	t	exact value	approximation	error
-0.2000	2	0.241701111254	0.241701111067	0.187E-09
0.0000	2	0.375668941931	0.375668941588	0.343E-09
0.2000	2	0.523215078618	0.523215078096	0.522E-09
0.4000	2	0.668323882248	0.668323881517	0.732E-09
0.6000	2	0.786080733070	0.786080732090	0.980E-09
0.8000	2	0.839219032083	0.839219030806	0.128E-08
1.0000	2	0.773578882908	0.773578881325	0.158E-08
1.2000	2	0.636739215551	0.636739214238	0.131E-08

Table 6: Exact, approximated values and absolute error for the solution of (4.11) 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 $a_s = s$.

- [18] V. Maz'ya and G. Schmidt, Approximate Approximations, Math. Surveys and Monographs, vol. 141, AMS 2007.
- [19] V. Maz'ya, Sobolev spaces with applications to elliptic partial differential equations, vol. 342, Springer, 2011.
- [20] H. Takahasi and M. Mori, Doubly exponential formulas for numerical integration, Publ. RIMS, Kyoto Univ. 9 (1974), 721-741
- [21] J. Waldvogel, Towards a general error theory of the trapezoidal rule, in: Approximation and Computation, in: Springer Optim. Appl., vol. 42, Springer, New York, 2011, pp. 267282.

h^{-1}	τ^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
10	10	0.372E-02		0.249E-04		0.830E-07	
20	20	0.928E-03	2.00	0.155E-05	4.00	0.129E-08	6.00
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

Table 7: Exact, approximated values and rate for $\mathcal{H}_{[-1,1]}^{(0,0)} f_2(0.2, 1)$ using $\tilde{\mathcal{H}}_{0.0125,0.0125}^{(3,3)}$ and $\tilde{w} = w$, $\tilde{v} = v$.

h^{-1}	τ^{-1}	$M = 1$		$M = 2$		$M = 3$	
		error	rate	error	rate	error	rate
10	10	0.450E-02		0.246E-04		0.816E-07	
20	20	0.124E-02	1.99	0.154E-05	3.99	0.128E-08	5.98
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 8: Exact, approximated values and rate for $\mathcal{H}_{[-1,1]}^{(0,0)} f_2(0.2, 1)$ using $\tilde{\mathcal{H}}_{0.0125,0.0125}^{(3,3)}$ and the Hestenes extension corresponding to $a_s = 1/s$.

		$n = 3$			$n = 10$	
x	t	exact value	approximation	error	approximation	error
-0.2	2	1.509084524073	1.509084524513	0.439E-09	1.509084526823	0.275E-08
0.0	2	2.000000000000	2.000000000713	0.713E-09	2.000000003735	0.374E-08
0.2	2	2.251289563841	2.251289564812	0.971E-09	2.251289568228	0.439E-08
0.4	2	2.105263013311	2.105263014485	0.117E-08	2.105263017766	0.445E-08
0.6	2	1.492679721280	1.492679722590	0.131E-08	1.492679725094	0.381E-08
0.8	2	0.576860208665	0.576860210112	0.145E-08	0.576860211331	0.267E-08
1.0	2	0.000000000000	0.00000001729	0.173E-08	0.00000001694	0.169E-08
1.2	2	0.000000000000	0.00000001057	0.106E-08	0.00000000584	0.584E-09
		$n = 100$			$n = 1000$	
x	t	exact value	approximation	error	approximation	error
-0.2	2	1.509084524073	1.509084552907	0.288E-07	1.509084812981	0.289E-06
0.0	2	2.000000000000	2.00000038297	0.383E-07	2.00000382975	0.383E-06
0.2	2	2.251289563841	2.251289607140	0.433E-07	2.251289995125	0.431E-06
0.4	2	2.105263013311	2.105263054196	0.409E-07	2.105263417014	0.404E-06
0.6	2	1.492679721280	1.492679751068	0.298E-07	1.492680008316	0.287E-06
0.8	2	0.576860208665	0.576860221795	0.131E-07	0.576860321260	0.113E-06
1.0	2	0.000000000000	0.00000001648	0.165E-08	0.00000001624	0.162E-08
1.2	2	0.000000000000	0.00000000052	0.515E-10	0.000000000000	0.281E-13

Table 9: Exact, approximated values and absolute errors for the solution of (4.11) with $f(\mathbf{x}, t)$ in (4.12) where $w(x) = e^x(x^2 - 1)$ and $v(t) = t$, at the point $(x, 0, \dots, 0, t) \in \mathbb{R}^n \times \mathbb{R}_+$ using $\tilde{\mathcal{H}}_{0.0125,0.0125}^{(3,3)}$ and the Hestenes extension corresponding to $a_s = 1/2^s$.

			$n = 10^4$	$n = 10^5$	$n = 10^6$	$n = 10^7$
x	t	exact value	error	error	error	error
-0.200	2	1.50908452	0.289E-05	0.289E-04	0.289E-03	0.289E-02
0.000	2	2.00000000	0.383E-05	0.383E-04	0.383E-03	0.383E-02
0.200	2	2.25128956	0.431E-05	0.431E-04	0.431E-03	0.432E-02
0.400	2	2.10526301	0.403E-05	0.403E-04	0.403E-03	0.404E-02
0.600	2	1.49267972	0.286E-05	0.286E-04	0.286E-03	0.286E-02
0.800	2	0.57686021	0.111E-05	0.110E-04	0.110E-03	0.111E-02
1.000	2	0.00000000	0.162E-08	0.161E-08	0.161E-08	0.161E-08

Table 10: Absolute errors for the solution of (4.11) with $f(\mathbf{x}, t)$ in (4.12) where $w(x) = e^x(x^2 - 1)$ and $v(t) = t$, at the point $(x, 0, \dots, 0, t) \in \mathbb{R}^n \times \mathbb{R}_+$ using $\tilde{\mathcal{H}}_{0.0125, 0.0125}^{(3,3)}$ and the Hestenes extension corresponding to $a_s = 1/2^s$.

	h^{-1}	τ^{-1}	$M = 1$		$M = 2$		$M = 3$	
			error	rate	error	rate	error	rate
$n = 3$	40	20	0.868E-02		0.252E-04		0.485E-07	
	80	40	0.221E-02	1.97	0.165E-05	3.93	0.824E-09	5.87
	160	80	0.558E-03	1.98	0.106E-06	3.96	0.134E-10	5.94
	320	160	0.140E-03	1.99	0.667E-08	3.98	0.210E-12	5.99
	640	320	0.355E-04	1.98	0.409E-09	4.02	0.130E-13	5.66
$n = 10$	40	20	0.268E-01		0.834E-04		0.171E-06	
	80	40	0.678E-02	1.98	0.523E-05	3.99	0.269E-08	5.99
	160	80	0.170E-02	1.99	0.327E-06	3.99	0.421E-10	5.99
	320	160	0.425E-03	1.99	0.205E-07	3.99	0.660E-12	5.99
	640	320	0.107E-03	1.99	0.127E-08	4.01	0.142E-13	5.54
$n = 10^2$	40	20	0.235E+00		0.840E-03		0.173E-05	
	80	40	0.658E-01	1.83	0.527E-04	3.99	0.271E-07	5.99
	160	80	0.169E-01	1.96	0.329E-05	3.99	0.423E-09	5.99
	320	160	0.426E-02	1.99	0.206E-06	3.99	0.664E-11	5.99
	640	320	0.107E-02	1.99	0.129E-07	4.00	0.135E-12	5.61
$n = 10^3$	40	20	0.847E+00		0.837E-02		0.173E-04	
	80	40	0.477E+00	0.82	0.330E-04	3.99	0.271E-06	5.99
	160	80	0.156E+00	1.61	0.527E-03	3.99	0.424E-08	5.99
	320	160	0.418E-01	1.89	0.206E-05	3.99	0.664E-10	5.99
	640	320	0.106E-01	1.97	0.129E-06	4.00	0.121E-11	5.77
$n = 10^4$	40	20	0.888E+00		0.803E-01		0.173E-03	
	80	40	0.888E+00	0.00	0.526E-02	3.93	0.271E-05	5.99
	160	80	0.759E+00	0.22	0.330E-03	3.99	0.424E-07	5.99
	320	160	0.340E+00	1.16	0.206E-04	3.99	0.663E-09	5.99
	640	320	0.101E+00	1.75	0.129E-05	3.99	0.120E-10	5.78
$n = 10^5$	40	20	0.888E+00		0.544E+00		0.173E-02	
	80	40	0.888E+00	0.00	0.512E-01	3.40	0.271E-04	5.99
	160	80	0.888E+00	0.00	0.329E-02	3.95	0.424E-06	5.99
	320	160	0.881E+00	0.01	0.206E-03	3.99	0.653E-08	6.01
	640	320	0.622E+00	0.50	0.129E-04	3.99	0.904E-10	6.17
$n = 10^6$	40	20	0.888E+00		0.888E+00		0.171E-01	
	80	40	0.888E+00	0.00	0.398E+00	1.15	0.271E-03	5.98
	160	80	0.888E+00	0.00	0.324E-01	3.61	0.423E-05	6.00
	320	160	0.888E+00	0.00	0.206E-02	3.97	0.607E-07	6.12
	640	320	0.888E+00	0.00	0.129E-03	3.99	0.120E-08	5.66
$n = 10^7$	40	20	0.888E+00		0.888E+00		0.157E+00	
	80	40	0.888E+00	0.00	0.886E+00	0.00	0.271E-02	5.86
	160	80	0.888E+00	0.00	0.276E+00	1.68	0.423E-04	6.00
	320	160	0.888E+00	0.00	0.204E-01	3.75	0.568E-06	6.21
	640	320	0.888E+00	0.00	0.129E-02	3.98	0.654E-07	3.11

Table 11: Absolute errors and approximation rates for the solution of (4.11) with $f(\mathbf{x}, t)$ in (4.12) where $w(x) = \cos^2(\pi x/2)$ and $v(t) = 1 - e^{-t}$, at the point $\mathbf{x} = (0.2, 0, \dots, 0)$; $t = 4$ using $\tilde{\mathcal{H}}_{h,\tau}^{(M,M)}$ and the Hestenes extension corresponding to $a_s = 1/s$.