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# Numerical treatment of retarded boundary integral equations by sparse panel clustering

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We consider the wave equation in a boundary integral formulation. The discretization in time is done by using convolution quadrature techniques and a Galerkin boundary element method for the spatial discretization. In a previous paper, we have introduced a sparse approximation of the system matrix by cut-off, in order to reduce the storage costs. In this paper, we extend this approach by introducing a panel clustering method to further reduce these costs.

*Keywords*: boundary integral equations; wave equation; convolution quadrature; panel clustering.

## 1. Introduction

When discretizing the wave equation, one has the choice of treating this partial differential equation directly or to transform it into a boundary integral equation. In this paper, we consider the formulation as a boundary integral equation with a retarded potential which goes back to the early 1960s (see Friedman & Shaw, 1962). One advantage of this approach is seen when considering an exterior problem, i.e. when the spatial domain is unbounded. The treatment of problems on unbounded domains using the original formulation usually requires a restriction to an artificial finite domain, together with some additional non-reflecting boundary conditions. In contrast, the boundary integral equation is formulated on the (lower dimensional) bounded surface of the domain. No artificial boundary conditions are necessary. An additional advantage is the reduction of the dimension of the problem by one: if we consider a 3D problem and denote by $h$ a typical mesh size in the spatial discretization, the boundary integral equation leads to $\mathrm{O}(h^{-2})$ unknowns instead of $\mathrm{O}(h^{-3})$, and, correspondingly, much smaller linear systems have to be solved. A drawback of the boundary integral formulation is the fact that the corresponding matrices are densely populated. This leads to a (at least) quadratic complexity. For potential problems of elliptic type, fast methods (panel clustering, wavelets, multipole, $\mathscr{H}$-matrices) have been developed which reduce such costs to almost linear (linear up to a logarithmic factor) complexity. In this paper, we develop a panel clustering method for retarded boundary integral operators.

A way to discretize the wave equation in time is the convolution quadrature method (Lubich, 1988a, 1994). In Hackbusch *et al.* (2005, 2007), we have introduced two advanced versions of the method in

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order to reduce its complexity. In Hackbusch *et al.* (2005), a sparse approximation technique has been developed, where a simple cut off criterion allows to replace the original system matrices by sparse approximations. By using a panel clustering technique, the storage consumptions can be further reduced. In order to analyse the panel clustering approximation, estimates for the derivatives of the kernel functions in the boundary integral equation formulation are required. These estimates are developed in the present paper.

The paper is organized as follows: In Sections 2 and 3, we formulate the boundary integral equation and its discretization by using convolution quadrature in time and a Galerkin boundary element method in space. In Section 4, we recall the sparse approximation of the Galerkin matrices introduced in Hackbusch *et al.* (2005). In Section 5, we consider a panel clustering approximation to further reduce the storage and computational cost. To obtain error estimates, an analysis of the kernel functions and their derivatives is required. The necessary bounds are derived in Section 6.

There exist alternative numerical discretization methods which include collocation methods with some stabilization techniques (cf. Birgisson *et al.*, 1999; Bluck & Walker, 1996; Davies, 1994, 1997; Davies & Duncan, 2004; Miller, 1987; Rynne & Smith, 1990) and Laplace–Fourier methods coupled with Galerkin boundary elements in space (Bamberger & Ha-Duong, 1986; Costabel, 1994; Ding *et al.*, 1989; Ha-Duong, 2003). Numerical experiments can be found, e.g. in Ha-Duong *et al.* (2003).

In Ergin *et al.* (2000), a fast version of the 'marching-on-in-time' method is presented, which is based on a suitable plane wave expansion of the arising potential which reduces the storage and computational costs.

Our method is similar and shares some properties (the need to solve a series of elliptic problems) of certain methods for parabolic equations; see Hohage & Sayas (2005) and Sheen *et al.* (2003). A related, interesting variation of the convolution quadrature for convolution kernels whose Laplace transform is sectorial can be found in Schädle *et al.* (2006).

Another method which is also based on the convolution quadrature is presented in Banjai & Sauter (2007), where the major part of the solution process is carried out in the discrete Laplace image.

## 2. Boundary integral formulation

In this paper, we consider the numerical solution of the 3D wave equation. For this, let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain with boundary $\Gamma$. We consider the homogeneous wave equation

$$\partial_t^2 u(x,t) - \Delta u(x,t) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T),$$

with zero initial condition

$$u(x,0) = \partial_t u(x,0) = 0 \quad \text{for } x \in \Omega$$

and Dirichlet boundary conditions

$$u(x,t) = g(x,t) \quad \text{on } \Gamma \times (0,T).$$

To formulate the problem as a boundary integral equation, $u(x,t)$ can be written as a 'single-layer potential':

$$u(x,t) = \int_0^t \int_\Gamma \frac{\delta(t) - \tau - \|x-y\|}{4\pi \|x-y\|} \phi(y,\tau) \mathrm{d}s_y \, \mathrm{d}\tau,$$

$\delta(t)$ being the Dirac delta distribution. Taking the limit $x \to \Gamma$, we obtain the following boundary integral equation for the unknown density $\phi$:

$$\int_0^t \int_\Gamma k(\|x-y\|, t-\tau) \phi(y,\tau) \mathrm{d}s_y \, \mathrm{d}\tau = g(x,t) \quad \forall\, (x,t) \in \Gamma \times (0,T) \tag{2.1}$$

with the kernel function

$$k(d,t)=\frac{\delta(t-d)}{4\pi d}.$$

## 3. Convolution quadrature method

A time discretization of (2.1) can be obtained by introducing a step size $\Delta t$ and a maximal number of time steps $N$ and replacing the time convolution in (2.1) at time step $t_n = n\Delta t$ by a discrete convolution:

$$\sum_{j=0}^{n}\int_{\Gamma}\omega_{n-j}^{\Delta t}(\|x-y\|)\phi(y,t_j)\mathrm{d}s_y=g(x,t_n)\quad\forall x\in\Gamma,\ \ 1\leqslant n\leqslant N, \tag{3.1}$$

with convolution weights $\omega_n^{\Delta t}(d)$.

We use the convolution quadrature method (Lubich, 1988a, 1994) to obtain the suitable weights $\omega_n^{\Delta t}(d)$. This method is based on a linear multistep method and inherits its stability properties. For the derivation of the convolution quadrature method, we refer to Hackbusch *et al.* (2005, 2007) and Lubich (1994). Here, we only give the definition of the quadrature weights.

DEFINITION 3.1 Let

$$\sum_{j=0}^{k}\alpha_j u^{n+j-k}=\Delta t\sum_{j=0}^{k}\beta_j f(u^{n+j-k}) \tag{3.2}$$

be a linear multistep method for an ordinary differential equation $u'(t)=f(u(t))$, where $u^n\approx u(t_n)$. Define

$$\gamma(\zeta):=\frac{\sum_{j=0}^{k}\alpha_j\zeta^{k-j}}{\sum_{j=0}^{k}\beta_j\zeta^{k-j}}$$

as the quotient of its generating polynomials.

DEFINITION 3.2 Given a linear multistep method (3.2), the ‘convolution weights’ $\omega_n^{\Delta t}(d)$ of the convolution quadrature method are the expansion coefficients in the formal power series

$$\hat{k}\left(d,\frac{\gamma(\zeta)}{\Delta t}\right)=\sum_{n=0}^{\infty}\omega_n^{\Delta t}(d)\zeta^n,$$

where $\hat{k}(d,s):=\frac{\mathrm{e}^{-sd}}{4\pi d}$ is the Laplace transform of the kernel function $k(d,t)=\frac{\delta(t-d)}{4\pi d}$ in (2.1).

The convolution weights can be derived by the Taylor expansion:

$$\omega_n^{\Delta t}(d)=\frac{1}{n!}\partial_\zeta^n\,\hat{k}\left(d,\frac{\gamma(\zeta)}{\Delta t}\right)\bigg|_{\zeta=0}.$$

Throughout this paper, we consider the second-order accurate, $A$-stable BDF2 scheme, with

$$\gamma(\zeta)=\frac{1}{2}(\zeta^2-4\zeta+3).$$

In that case, using the formula for multiple differentiation of composite functions (see, e.g. Gradshteyn & Ryzhik, 1965), we obtain the explicit representation

$$\omega_n^{\Delta t}(d) = \frac{1}{n!}\frac{1}{4\pi d}\left(\frac{d}{2\Delta t}\right)^{n/2} \mathrm{e}^{-\frac{3d}{2\Delta t}} H_n\left(\sqrt{\frac{2d}{\Delta t}}\right),$$

where $H_n$ are the Hermite polynomials.

The convergence rate and stability properties of the convolution quadrature method are inherited by the linear multistep method, i.e. if (3.2) is $A$-stable and second-order accurate, then so is (3.1). Stability and convergence results for the semi-discrete problem can be found in Hackbusch *et al.* (2005) and Lubich (1994).

For the space discretization, we employ a Galerkin boundary element method. For this, we consider a boundary element space, e.g. of piecewise constant or piecewise linear functions, and a basis $(b_i(x))_{i=1}^M$. For the Galerkin boundary element method, we replace $\phi(y, t_j)$ in (3.1) by

$$\phi^j_{\Delta t,h}(y) = \sum_{i=1}^M \boldsymbol{\phi}_{j,i} b_i(y)$$

and impose the integral equation in a weak form:

$$\sum_{j=0}^n \sum_{i=1}^M \phi_{j,i} \int_\Gamma \int_\Gamma \omega^{\Delta t}_{n-j}(x-y) b_i(y) b_k(x) \mathrm{d}s_y \, \mathrm{d}s_x = \int_\Gamma g(x, t_n) b_k(x) \mathrm{d}s_x$$

for all $1 \leqslant k \leqslant M$ and $n = 1, \ldots, N$. This can be written as a linear system

$$\sum_{j=0}^n \mathbf{A}_{n-j}\phi_j = \mathbf{g}_n, \quad n = 1, \ldots, N, \tag{3.3}$$

with

$$(\mathbf{A}_{n-j})_{k,i} := \int_\Gamma \int_\Gamma \omega^{\Delta t}_{n-j}(x-y) b_i(y) b_k(x) \mathrm{d}s_y \, \mathrm{d}s_x$$

and

$$(\mathbf{g}_n)_k = \int_\Gamma g(x, n\Delta t) b_k(x) \mathrm{d}s_x.$$

The compact formulation as a block triangular system is given by

$$\overrightarrow{\mathbf{A}}_N \overrightarrow{\boldsymbol{\phi}}_N = \overrightarrow{\mathbf{g}}_N, \tag{3.4}$$

where the block matrix $\overrightarrow{\mathbf{A}}_N \in \mathbb{R}^{NM} \times \mathbb{R}^{NM}$ and the vector $\overrightarrow{\mathbf{g}}_N \in \mathbb{R}^{NM}$ are defined by

$$\overrightarrow{\mathbf{A}}_N := \begin{pmatrix} \mathbf{A}_0 & \mathbf{0} & \cdots & & & \mathbf{0} \\ \mathbf{A}_1 & \mathbf{A}_0 & \ddots & & & \vdots \\ \mathbf{A}_2 & \mathbf{A}_1 & \ddots & & & \\ \vdots & \mathbf{A}_2 & \ddots & & \ddots & \\ & & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{A}_N & \cdots & & \mathbf{A}_2 & \mathbf{A}_1 & \mathbf{A}_0 \end{pmatrix} \quad \text{and} \quad \overrightarrow{\mathbf{g}}_N := \begin{pmatrix} \mathbf{g}_0 \\ \mathbf{g}_1 \\ \vdots \\ \mathbf{g}_N \end{pmatrix}. \tag{3.5}$$

The matrices $\mathbf{A}_j$ have dimension $M \times M$ and are fully populated. The following simple procedure is the algorithmic formulation of (3.4):

procedure solve;
begin
for $i := 0$ to $N$ do begin
$\mathbf{s} := \mathbf{g}_i$;
for $j := 0$ to $i - 1$ do

$$\mathbf{s} := \mathbf{s} - \mathbf{A}_{i-j}\boldsymbol{\phi}_j \tag{3.6}$$

solve

$$\mathbf{A}_0\boldsymbol{\phi}_i = \mathbf{s}; \tag{3.7}$$

end; end;

The solution of the system $\mathbf{A}_0\phi_i = \mathbf{s}$ should be realized by means of an iterative solver.

## 4. Sparse approximation by cut-off

The matrices in (3.3) are densely populated. This is due to the fact that, although the basis functions have local support, they are coupled by the non-local convolution coefficients $\omega_n^{\Delta t}(d)$. In Hackbusch *et al.* (2005), we have introduced a sparse approximation of the matrices $\mathbf{A}_n$ to reduce the storage requirements. To find such an approximation, we investigate the convolution coefficients $\omega_n^{\Delta t}(d)$. Although they are non-local functions, they can be replaced by more localized functions. In Fig. 1, $\omega_{100}^1(d)$ and $\omega_{200}^1(d)$ are shown. The functions $\omega_n^{\Delta t}(d)$ have their maximum at about $d = n\Delta t$ and outside an interval of width $\mathrm{O}(\Delta t\sqrt{n})$, they are small enough to be replaced by 0. In Hackbusch *et al.* (2005), the following results are shown.

LEMMA 4.1 Let

$$I_{n,\varepsilon}^{\Delta t} := \begin{cases} \left[0, \frac{2}{3}\Delta t|\log\varepsilon|\right], & n = 0, \\ [t_n - 3\Delta t\sqrt{n}|\log\varepsilon|, t_n + 3\Delta t\sqrt{n}|\log\varepsilon|] \cap \operatorname{diam}(\Omega), & n > 0. \end{cases} \tag{4.1}$$

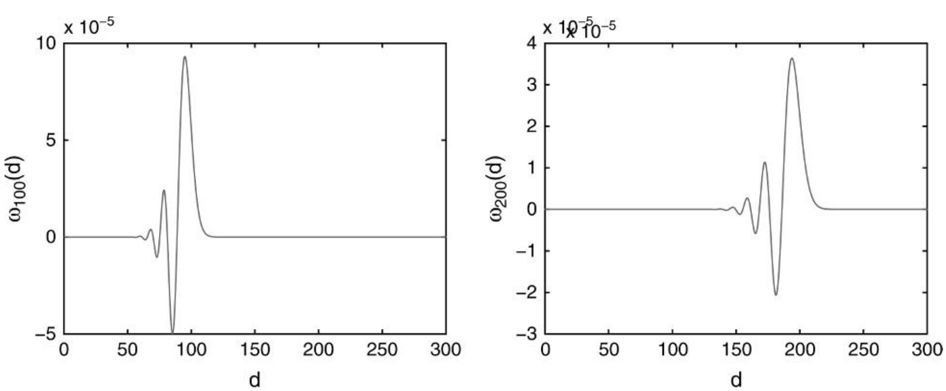


FIG. 1. Convolution weight $\omega_n^{\Delta t}(d)$, $n = 100$, $n = 200$, $\Delta t = 1$.

Then, there holds

$$|\omega_n^{\Delta t}(d)| \leqslant \frac{\varepsilon}{4\pi d} \quad \forall\, d \notin I_{n,\varepsilon}^{\Delta t}. \tag{4.2}$$

Replacing $\omega_n^{\Delta t}(d)$ by zero, outside the interval $I_{n,\varepsilon}^{\Delta t}$ leads to the following sparse approximation.

DEFINITION 4.2 For a given error tolerance $\varepsilon$, let

$$\mathscr{P}_{\varepsilon,n} := \{(i, j) \mid \exists\, (x, y) \in \operatorname{supp}(b_i) \cap \operatorname{supp}(b_j)\colon \|x - y\| \in I_{n,\varepsilon}^{\Delta t}\}.$$

The sparse approximation $\tilde{\mathbf{A}}_n$ is obtained by setting

$$(\tilde{\mathbf{A}}_n)_{i,j} := \begin{cases} (\mathbf{A}_n)_{i,j}, & \text{if } (i, j) \in \mathscr{P}_{\varepsilon,n}, \\ 0, & \text{otherwise.} \end{cases}$$

The solutions of the algebraic system

$$\sum_{j=0}^{n} \tilde{\mathbf{A}}_{n-j} \tilde{\boldsymbol{\phi}}_j = \mathbf{g}_n, \quad n = 1, \ldots, N, \tag{4.3}$$

are the coefficient vectors of the approximate Galerkin solutions

$$\tilde{\phi}_{\Delta t,h}^n := \sum_{i=1}^{M} \tilde{\boldsymbol{\phi}}_{n,i} b_i.$$

The following theorem follows directly from Hackbusch *et al.* (2005, Theorem 4.7) by using $\frac{1-\mathrm{e}^{-\sigma \Delta t}}{2c_{\Delta} c_{\sigma}} \leqslant C\Delta t$ therein.

THEOREM 4.3 Assume that the exact solution $\phi(\cdot, t)$ is in $H^{m+1}(\Gamma)$ for any $t \in [0, T]$. There exists a constant $C > 0$ such that for all $0 < \varepsilon < Ch\Delta t^3$, the approximate Galerkin solutions $\tilde{\phi}_{\Delta t,h}^n$ exist and satisfy the error estimate

$$\|\tilde{\phi}_{\Delta t,h}^n - \phi(\cdot, t)\|_{H^{-1/2}(\Gamma)} \leqslant C_g(T)(\varepsilon h^{-1} \Delta t^{-5} + \Delta t^2 + h^{m+3/2}). \tag{4.4}$$

REMARK 4.4 The choice

$$\Delta t^2 \sim h^{m+3/2} \quad \text{and} \quad \varepsilon \sim (\Delta t)^7 h \sim h^{7m/2+25/4} \tag{4.5}$$

balances the three error terms in (4.4).

The storage cost for the matrix $\tilde{\mathbf{A}}_n$ is given by

$$\mathrm{O}\left(M \max\left\{1, t_n^{\frac{3}{2}} \sqrt{\Delta t} M \log M\right\}\right) \tag{4.6}$$

and some cases are summarized in Table 1, assuming that $\Delta t^2 \sim h^{m+\frac{3}{2}}$. The total storage amount follows by summing (4.6) for $n = 0, 1, \ldots, N$. By using $(N\Delta t)^2 \sim 1$ and $M \geqslant \mathrm{O}(N)$, we obtain

$$\text{the total storage amount for all } \tilde{\mathbf{A}}_n,\ 0 \leqslant n \leqslant N: \quad \mathrm{O}(N^{1/2} M^2 \log M).$$

This is a significant reduction of the storage cost by a factor of $\mathrm{O}(N^{1/2})$ compared to the original Galerkin method where the storage cost is $\mathrm{O}(NM^2)$.

TABLE 1 *Storage requirements for* $\tilde{\mathbf{A}}_n$

| | $m = 0$ | $m = 1$ |
|---|---|---|
| $n = \mathrm{O}(\log M)$ | $CM^{1+\frac{1}{4}}\log^{5/2} M$ | $CM$ |
| $n = \mathrm{O}(N)$ | $Ct_n^{3/2}M^{1+\frac{13}{16}}\log M$ | $Ct_n^{3/2}M^{1+\frac{11}{16}}\log M$ |

REMARK 4.5 In Hairer *et al.* (1985) and Lubich (1988a,b, 1994), FFT techniques have been introduced to solve the system (3.4). While the storage costs stay unchanged $\mathrm{O}(NM^2)$, the computational complexity is reduced from $\mathrm{O}(N^2M^2)$ to $\mathrm{O}(N\log^2 NM^2)$. Our cut off strategy reduces the storage cost to $\mathrm{O}(N^{1/2}M^2)$, while the computational complexity is reduced less significantly. However, the use of panel clustering (cf. Section 5) will further reduce the computational complexity of our approach, see Remark 5.10.

The subroutine 'procedure solve' (cf. Section 3) can easily be modified to take into account the sparse approximation by replacing step (3.6) by

$$\text{for all } 1 \leqslant k \leqslant M\colon \quad s_k := s_k - \sum_{\ell:(k,\ell)\in\mathscr{P}_{\varepsilon,i-j}} (\mathbf{A}_{i-j})_{k,\ell}\phi_{j,\ell}, \tag{4.7}$$

while the iterative solution of (3.7) should take into account the sparsity of $\tilde{\mathbf{A}}_0$ as well.

## 5. Panel clustering

The panel clustering method was developed in Hackbusch & Nowak (1989) for the data-sparse approximation of boundary integral operators which are related to elliptic boundary-value problems. Since then, the field of sparse approximation of non-local operators has grown rapidly and nowadays advanced versions of the panel clustering method are available and a large variety of alternative methods such as wavelet discretizations, multipole expansions, $\mathscr{H}$-matrices etc. exists. However, these fast methods (with the exception of $\mathscr{H}$-matrices) are developed mostly for problems of elliptic type, while the data-sparse approximation of retarded potentials is to our knowledge still in its infancies. In this section, we develop the panel clustering method for retarded potentials.

### 5.1 *The algorithm*

If we employ the cut off strategy as in Section 4, a matrix–vector multiplication $\tilde{\mathbf{A}}_n\boldsymbol{\phi}$ with a vector $\boldsymbol{\phi} = (\phi_i)_{i=1}^M \in \mathbb{R}^M$ can be written in the form

$$\forall\, 1 \leqslant k \leqslant M\colon \quad (\tilde{\mathbf{A}}_n\phi)_k = \sum_{\ell:(k,\ell)\in\mathscr{P}_{\varepsilon,n}} \phi_\ell \int_\Gamma\int_\Gamma \omega_n^{\Delta t}(\|x-y\|)b_\ell(y)b_k(x)\,\mathrm{d}\Gamma_y\,\mathrm{d}\Gamma_x. \tag{5.1}$$

For the application of the panel clustering algorithm, the set $\mathscr{P}_{\varepsilon,n}$ is split into admissible blocks which we are going to explain next. The panel clustering method will be applied as soon as

$$n > n^{\mathrm{pc}} := C\max\left\{\log^2 M,\, M^{m-\frac{1}{2}}\log^4 M\right\} \tag{5.2}$$

for some constant $C$. For $n < n^{\mathrm{pc}}$, it will turn out that, for the simple cut off strategy, the complexity has the same asymptotic behaviour. (Note that for the first time steps, the simple cut off strategy reduces the complexity much more significantly than for the later time steps, see Table 1.)

Let $\mathbb{N}_M := \{1, 2, \ldots, M\}$.

DEFINITION 5.1 A 'cluster' $c$ is a subset of $\mathbb{N}_M$. If $c$ is a cluster, the corresponding subdomain of $\Gamma$ is $\Gamma_c := \cup_{i \in t} \operatorname{supp}(b_i)$. The 'cluster box' $Q_c \subset \mathbb{R}^3$ is the minimal axis-parallel cuboid which contains $\Gamma_c$ and the 'cluster size' $L_c$ is the maximal side length of $Q_c$.

DEFINITION 5.2 Let $\varepsilon > 0$ and $n > n^{\mathrm{pc}}$. Let $\eta > 0$ be some control parameter. A pair of clusters $(c, s) \subset \mathbb{N}_M \times \mathbb{N}_M$ is 'admissible' at time step $t_n$ if

$$\max\{L_c, L_s\} \leqslant \eta \frac{\Delta t n^b}{|\log \varepsilon|}. \tag{5.3}$$

The power $b$ in (5.3) is a fixed number. Some comments are given in Remark 5.3.

REMARK 5.3 In Sections 5.2 and 6, we will prove that the choice $b = 1/4$ preserves the optimal convergence order of the unperturbed discretization (without panel clustering and cut-off). However, a larger value of $b$ would improve the complexity estimates because, then, more blocks are admissible for panel clustering. Numerical experiments indicate that a slightly increased value $b \approx 0.3$ preserves the optimal convergence rates as well. In this light, we assume for some technical estimates that $b$ in (5.3) satisfies

$$0.25 \leqslant b \leqslant 0.3. \tag{5.4}$$

The panel clustering method starts by constructing a set $\mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}$ which consists of admissible, pairwise disjoint pairs of clusters such that

$$(c, s) \cap \mathscr{P}_{\varepsilon,n} \neq \emptyset$$

and

$$\mathscr{P}_{\varepsilon,n} \subset \bigcup_{(c,s) \in \mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}} (c, s).$$

We skip here the explicit formulation of the divide-and-conquer algorithm for the efficient construction of $\mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}$ by introducing a tree structure for the clusters but refer, e.g. to Sauter & Schwab (2004) for the details.

Expression (5.1) becomes

$$(\tilde{\mathbf{A}}_n \phi)_k = \sum_{(c,s) \in \mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}} \sum_{\ell:(k,\ell) \in (c,s)} \phi_\ell \int_{\Gamma_c} \int_{\Gamma_s} \omega_n^{\Delta t}(\|x - y\|) b_\ell(y) b_k(x) \mathrm{d}\Gamma_y \, \mathrm{d}\Gamma_x. \tag{5.5}$$

The kernel function $\omega_n^{\Delta t}$ is now approximated on $\Gamma_c \times \Gamma_s$ by a separable expansion as follows: since $\omega_n^{\Delta t}(\|x - y\|)$ is defined on $Q_c \times Q_s$, we may define an approximation by Čebyšev interpolation:

$$\omega_n^{\Delta t}(\|x - y\|) \approx \check{\omega}_n^{\Delta t}(\|x - y\|) = \sum_{\mu,\nu \in (\mathbb{N}_q)^3} \mathscr{L}_c^{(\mu)}(x) \mathscr{L}_s^{(\nu)}(y) \omega_n^{\Delta t}(\|x^\mu - y^\nu\|), \tag{5.6}$$

where $\mathscr{L}_c^{(\mu)}$ and $\mathscr{L}_s^{(\nu)}$, respectively, are the tensorized versions of the $q$th-order Lagrange polynomials (properly scaled and translated to $Q_c$ and $Q_s$, respectively) corresponding to the tensorized Čebyšev nodes $x^\mu$ and $y^\nu$ for $Q_c$ and $Q_s$, respectively. Replacing the kernel functions $\omega_n^{\Delta t}$ under the integral in (5.5) allows to perform the integration with respect to $x$ and $y$ separately. This leads to

$$\sum_{\ell:(k,\ell)\in(c,s)} \phi_\ell \int_{\Gamma_c}\int_{\Gamma_s} \omega_n^{\Delta t}(\|x-y\|) b_\ell(y) b_k(x) \mathrm{d}\Gamma_y\, \mathrm{d}\Gamma_x$$
$$\approx \sum_{\ell:(k,\ell)\in(c,s)} \sum_{\mu,\nu\in(\mathbb{N}_q)^3} \mathbf{V}_c^{(\mu,k)} \mathbf{S}_{(c,s)}^{\mu,\nu} \mathbf{V}_s^{(\nu,\ell)} \phi_\ell,$$

where

$$\mathbf{V}_c^{(\mu,k)} := \int_{\Gamma_c} \mathscr{L}_c^{(\mu)}(x) b_k(x) \mathrm{d}\Gamma_x \quad \text{and} \quad \mathbf{S}_{(c,s)}^{\mu,\nu} := \omega_n^{\Delta t}(\|x^\mu - y^\nu\|). \tag{5.7}$$

Hence, the panel clustering approximation of (3.6) is given by replacing step (3.6) by

$$s_k := s_k - \sum_{(c,s)\in\mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}} \sum_{\ell:(k,\ell)\in(c,s)} \sum_{\mu,\nu\in(\mathbb{N}_q)^3} \mathbf{V}_c^{(\mu,k)} \mathbf{S}_{(c,s)}^{\mu,\nu} \mathbf{V}_s^{(\nu,\ell)} \phi_\ell. \tag{5.8}$$

Remember that for the first time steps, the matrices $\mathbf{A}_n$ are approximated using the simple cut off strategy.

REMARK 5.4 To guarantee the existence of admissible clusters, we need at least the smallest cluster pairs consisting of the support of the basis functions $b_i$ to be admissible.

For $m = 0$, we require (according to (4.5))

$$\eta \frac{\Delta t n^b}{|\log \varepsilon|} = \mathrm{O}\left(\eta \frac{h^{3/4} n^b}{|\log h|}\right) \geqslant \mathrm{O}(h) = L_{\{i\}}$$

which is always satisfied.

For $m = 1$, we get (with $b = 1/4$)

$$\eta \frac{\Delta t n^b}{|\log \varepsilon|} = \mathrm{O}\left(\eta \frac{h^{5/4} n^b}{|\log h|}\right) = \mathrm{O}\left(\eta \frac{h}{|\log h|}(hn)^{1/4}\right).$$

Hence, the condition

$$n \geqslant C M^{1/2} \log^4 M = \mathrm{O}(h^{-1}|\log h|^4)$$

ensures $\eta \frac{\Delta t n^b}{|\log \varepsilon|} \geqslant Ch$. Note that this is guaranteed by (5.2).

Although the admissibility criterion (5.3) differs from the standard criterion for elliptic boundary-value problems, the algorithmic formulation of the panel clustering is as in the elliptic case and, hence, is described in numerous papers; see, e.g. Sauter & Schwab (2004) and we do not recall the details here.

### 5.2 *Error analysis*

We proceed with the error analysis of the resulting perturbed Galerkin discretization which leads to an *a priori* choice of the interpolation order $q$ such that the convergence rate of the unperturbed discretization is preserved.

Standard estimates for tensorized Čebyšev interpolation yield

$$\sup_{z\in Q_c-Q_s} |\omega_n^{\Delta t}(\|z\|) - \check{\omega}_n^{\Delta t}(\|z\|)| \leqslant C\frac{L^{q+1}(1+\log^5 q)}{2^{2q+1}(q+1)!} \max_{i\in\{1,2,3\}} \sup_{z\in Q_c-Q_s} \left|\partial_{z_i}^{q+1}\omega(\|z\|)\right|,$$

where $C > 0$ is some constant independent of all parameters, $L$ denotes the maximal side length of the boxes $Q_c$ and $Q_s$ and $Q_c - Q_s$ is the difference domain $\{x - y : (x, y) \in Q_c \times Q_s\}$.

THEOREM 5.5 For $(c, s) \in \mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}$, assume that the partial derivatives of $\omega_n^{\Delta t}(\|x - y\|)$ satisfy

$$\max_{1\leqslant i\leqslant 3} \left|\partial_{z_i}^{q}\omega_n^{\Delta t}(\|z\|)\right| \leqslant q!\|z\|^{-1}\left(\frac{C\lambda}{\Delta t n^b}\right)^q \quad \forall z \in Q_c - Q_s. \tag{5.3a}$$

Then,

$$|\check{\omega}_n^{\Delta t}(\|x-y\|) - \omega_n^{\Delta t}(\|x-y\|)| \leqslant \frac{C_1}{\mathrm{dist}(Q_c, Q_s)}\left(\frac{C_2\max\{L_c, L_s\}\lambda}{\Delta t n^b}\right)^{q+1}. \tag{5.3b}$$

The validity of assumption (5.3a) with $b$ as in Definition 5.2 and

$$\lambda := 2\eta + 3|\log\varepsilon| \tag{5.9}$$

will be derived in Theorem 6.6.

REMARK 5.6 Note that the panel clustering is applied on blocks $(c, s) \subset \mathscr{P}_{\varepsilon,n}$ which satisfy (5.3) and, hence there exists an $(x_0, y_0) \in \Gamma_c \times \Gamma_s$ such that

$$|\|x_0 - y_0\| - t_n| \leqslant \tilde{\lambda}\,\Delta t\sqrt{n} \quad \text{with } \tilde{\lambda} := 3|\log\varepsilon|.$$

As a consequence, we have for any $(x, y) \in \Gamma_c \times \Gamma_s$ (recall $b < 1/2$),

$$\begin{aligned} |\|x-y\| - t_n| &\leqslant |\|x-y\| - \|x_0-y_0\|| + \tilde{\lambda}\,\Delta t\sqrt{n} \leqslant L_c + L_s + \tilde{\lambda}\,\Delta t\sqrt{n} \\ &\leqslant (2\eta n^{b-1/2} + \tilde{\lambda})\Delta t\sqrt{n} \leqslant \lambda\,\Delta t\sqrt{n} \end{aligned}$$

with $\lambda$ as in (5.9).

THEOREM 5.7 Let $0 < \varepsilon < \frac{1}{8}$ and $n > 16|\log^2\varepsilon|$. Let the assumptions of Theorem 5.5 be satisfied and the interpolation order be chosen according to $q \geqslant |\log\varepsilon|/\log 2$. Let $(c, s) \in \mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}$ be admissible for some $0 < \eta \leqslant \eta_0$ and sufficiently small $\eta_0 = \mathrm{O}(1)$. Then,

$$|\check{\omega}_n^{\Delta t}(\|x-y\|) - \omega_n^{\Delta t}(\|x-y\|)| \leqslant C\frac{\varepsilon}{\|x-y\|} \quad \forall (x, y) \in \Gamma_c \times \Gamma_s \tag{5.10}$$

for some $C$ independent of $n$ and $\Delta t$.

*Proof.* Assume that $(c, s) \in \mathscr{P}_{\varepsilon,n}^{\mathrm{pc}}$. As derived above,

$$|\|x-y\| - t_n| \leqslant \frac{\lambda t_n}{\sqrt{n}} \quad \forall (x, y) \in \Gamma_c \times \Gamma_s.$$

Thus, if $\lambda < \sqrt{n}$, we have

$$t_n \leqslant \left(1 - \frac{\lambda}{\sqrt{n}}\right)^{-1} \|x - y\|.$$

We also have

$$\begin{aligned}\operatorname{dist}(Q_c, Q_s) &\geqslant \|x - y\| - \sqrt{3}(L_c + L_s) \geqslant \|x - y\| - 2\sqrt{3}\eta t_n n^{b-1} \\ &\geqslant \|x - y\| \left(1 - \frac{2\sqrt{3}\eta n^{b-1}}{1 - \frac{\lambda}{\sqrt{n}}}\right).\end{aligned}$$

Under the assumptions

$$n \geqslant 16|\log \varepsilon|^2 \tag{5.11}$$

and

$$\eta < \frac{|\log \varepsilon|}{4},$$

we have $\lambda < \sqrt{n}$ and obtain

$$\operatorname{dist}(Q_c, Q_s) \geqslant \|x - y\| \left(1 - \frac{\sqrt{3}}{2}|\log \varepsilon|^{-\frac{1}{2}}\right).$$

Assuming that $\varepsilon \leqslant \frac{1}{8}$, we obtain

$$\frac{1}{\operatorname{dist}(Q_c, Q_s)} \leqslant \frac{2}{\|x - y\|}. \tag{5.12}$$

Conditions (5.3) and (5.11) and the definition of $\lambda$ imply

$$\frac{C_2 \max\{L_c, L_s\}\lambda}{\Delta t n^b} \leqslant C_3 \eta.$$

Hence, from Theorem 5.5, we obtain the estimate

$$|\check{\omega}_n^{\Delta t}(\|x - y\|) - \omega_n^{\Delta t}(\|x - y\|)| \leqslant \frac{C_1}{\operatorname{dist}(Q_c, Q_s)} (C_3 \eta)^{q+1}.$$

Inserting (5.12) leads to

$$|\check{\omega}_n^{\Delta t}(\|x - y\|) - \omega_n^{\Delta t}(\|x - y\|)| \leqslant \frac{2C_1}{\|x - y\|} (C_3 \eta)^{q+1}.$$

Finally, the condition $\eta_0 \leqslant (2C_3)^{-1}$ implies that the interpolation order

$$q \geqslant \frac{|\log \varepsilon|}{\log 2}$$

leads to an approximation which satisfies

$$|\check{\omega}_n^{\Delta t}(\|x - y\|) - \omega_n^{\Delta t}(\|x - y\|)| \leqslant \frac{2C_1 \varepsilon}{\|x - y\|}.$$

□

In Hackbusch *et al.* (2005), an analysis of the Galerkin method has been derived which takes into account additional perturbations. Since it is only based on abstract approximations which satisfy an error estimate of type (5.10), we directly obtain a similar convergence theorem also for the panel clustering method. In the following, we denote by $\tilde{\phi}^n_{\Delta t,k}$ the solution at time $t_n$ of the Galerkin discretization with cut off strategy and panel clustering.

THEOREM 5.8 Let the assumption of Theorem 5.7 be satisfied. We assume that the exact solution $\phi(\cdot,t)$ is in $H^{m+1}(\Gamma)$ for any $t \in [0,T]$. Then, there exists a $C > 0$ such that for all cut off parameters $\varepsilon$ in (4.1), such that $0 < \varepsilon < Ch\Delta t^3$ and interpolation orders $q \geqslant |\log \varepsilon|/\log 2$, the solution $\tilde{\phi}^n_{\Delta t,h}$ with cut-off and panel clustering satisfies the error estimate

$$\|\tilde{\phi}^n_{\Delta t,h} - \phi(\cdot,t_n)\|_{H^{-1/2}(\Gamma)} \leqslant C_g(T)(\varepsilon h^{-1}\Delta t^{-5} + \Delta t^2 + h^{m+3/2}).$$

COROLLARY 5.9 Let the assumptions of Theorem 5.8 be satisfied. Let $\Delta t \sim h^{m+3/2}$ and choose $\varepsilon \sim h^{7m/2+25/4}$. Then, the solution $\tilde{\phi}_{\Delta t,h}$ exists and converges with the optimal rate

$$\|\tilde{\phi}^n_{\Delta t,h} - \phi(\cdot,t_n)\|_{H^{-1/2}(\Gamma)} \leqslant C_g(T)h^{m+3/2} \sim C_g(T)\Delta t^2.$$

### 5.3 *Complexity estimates*

In this subsection, we investigate the complexity of our sparse approximation of the wave discretization. We always employ the theoretical value $1/4$ for the exponent $b$ in (5.3) (cf. Remark 5.3).

5.3.1 *Sparse approximation of the system matrix* $\tilde{\mathbf{A}}_n$*.* To simplify the complexity analysis, we assume that only the simple cut off strategy and not the panel clustering method is applied for the first time steps:

$$0 \leqslant n \leqslant n^{\mathrm{pc}}. \tag{5.13}$$

By using (4.5) and (4.6), the number of non-zero entries of all $\tilde{\mathbf{A}}_n$ in the case (5.13) is estimated from above by $\mathrm{O}(NM^{\frac{7}{8}}\log^6 M)$ and $\mathrm{O}(NM^{1+\frac{3}{8}}\log^{11} M)$ for $m = 0$ and $m = 1$, respectively.

5.3.2 *Panel clustering.* The tree structure for the panel clustering algorithm has to be generated only once and, hence, the computational and storage complexity is negligible compared to the other steps of the algorithm. The entries of the matrices $\mathbf{V}$ (cf. (5.7)) are computed recursively by using the tree structure. The details can be found in Hackbusch *et al.* (2007) and Sauter & Schwab (2004). In Hackbusch *et al.* (2007), it is shown that the computational and storage complexity is negligible compared to the generation of the influence matrices $\mathbf{S}_{(c,s)}$ (cf. (5.7)).

5.3.3 *Computation of the influence matrices.* First, we compute the cardinality of $\mathscr{P}^{\mathrm{pc}}_{\varepsilon,n}$. Note that the maximal diameter of a cluster $c$ satisfying condition (5.3) is bounded by

$$L_c \leqslant \eta \frac{\Delta t n^b}{|\log \varepsilon|}. \tag{5.14}$$

An assumption on the cluster tree and the geometric shape of the surface is that

$$|\{(x,y) \in \Gamma \times \Gamma \mid \|x-y\| \in I^{\Delta t}_{n,\varepsilon}\}| = \mathrm{O}(\sqrt{\Delta t}t_n^{3/2}|\log \varepsilon|),$$

TABLE 2 *Storage requirements for the panel clustering approximation and sparse approximation*

| | Full-matrix representation | Cut off strategy | Panel clustering + Cut off strategy |
|---|---|---|---|
| $m=0$ | $\mathrm{O}(NM^2)$ | $\mathrm{O}\big(NM^{1+\frac{13}{16}}\log M\big)$ | $\mathrm{O}\big(NM^{1-\frac{1}{16}}\,\lvert\log M\rvert^{11}\big)$ |
| $m=1$ | $\mathrm{O}(NM^2)$ | $\mathrm{O}\big(NM^{1+\frac{11}{16}}\log M\big)$ | $\mathrm{O}\big(NM^{1+\frac{9}{16}}\,\lvert\log M\rvert^{11}\big)$ |

where $|\omega|$ denotes the area measure of some $\omega \subset \Gamma \times \Gamma$ (cf. Hackbusch *et al.*, 2007), and not only inequality (5.14) but also the reverse inequality holds for some other constant $\eta'$. Hence, for sufficiently small $\Delta t$, the number of pairs of clusters satisfying (5.3) is bounded by

$$\mathrm{O}\left(\frac{\sqrt{\Delta t}\, t_n^{3/2} |\log \varepsilon|}{\left(\eta' \frac{\Delta t n^b}{|\log \varepsilon|}\right)^4}\right). \tag{5.15}$$

The storage requirements per matrix $\mathbf{S}_{(c,s)}$ are given by $q^6 \sim |\log^6 \varepsilon|$ and this leads to a storage complexity of

$$\mathrm{O}\left(\frac{n^{3/2-4b} |\log \varepsilon|^{11}}{\eta'^4 \Delta t^2}\right). \tag{5.16}$$

Using the relations as in Corollary 5.9

$$\Delta t^2 \sim h^{m+3/2}, \quad \varepsilon \sim h^{7m/2+25/4}, \quad M = \mathrm{O}(h^{-2}),$$

we see that (5.16) is equivalent to (we use here $4b = 1$)

$$\mathrm{O}(n^{1/2} |\log M|^{11} M^{m/2+3/4}).$$

To compute the total storage cost, we sum over all $n \in \{n^{\mathrm{pc}}, \dots, N\}$ and obtain

$$\sum_{n=n^{\mathrm{pc}}}^{N} n^{\frac{1}{2}} |\log \varepsilon|^{11} M^{\frac{m}{2}+\frac{3}{4}} \leqslant C_1 N^{\frac{3}{2}} |\log M|^{11} M^{\frac{m}{2}+\frac{3}{4}} \leqslant C_2 N M^{\frac{5m}{8}+\frac{15}{16}} |\log M|^{11}$$
$$= C_2 \begin{cases} N M^{\frac{15}{16}} |\log M|^{11}, & m = 0, \\ N M^{1+\frac{9}{16}} |\log M|^{11}, & m = 1. \end{cases}$$

The total storage requirements are summarized in Table 2.

The table shows that the panel clustering method combined with the cut off strategy reduces the complexity of the space–time discretization of retarded integral equations significantly. For piecewise constant boundary elements, we get a storage complexity which behaves even better than linearly, i.e. $\mathrm{O}(NM)$.

REMARK 5.10

a. The panel clustering method is based on a twofold hierarchical structure:[1] The clusters are organized in a cluster tree and the expansion system on each cluster are polynomials. Hence, by

[1] In the context of $\mathscr{H}$-matrices, this twofold hierarchy is called $\mathscr{H}^2$-format.

elementary properties of polynomials, the expansion system on a cluster can be build from the expansion systems of the sons of the cluster. By employing this double hierarchy, the computational cost for a matrix–vector multiplication is proportional to the storage cost of the matrix (in the sparse panel clustering format).

b. Note that in the panel clustering regime ($n > n^{\mathrm{pc}}$), the integration of the highly oscillatory kernel functions is no longer necessary (cf. 5.8). Efficient quadrature methods for the integrals for $n < n^{\mathrm{pc}}$ is a topic of further research and we skip this aspect from the investigation of the computational costs here.

## 6. Estimate of the derivatives of the convolution coefficients

In Section 5, to obtain suitable error estimates, bounds for the derivatives of $\omega_n^{\Delta t}(\|x-y\|)$ were required. In this section, we derive such bounds and estimates on $b$ in Theorem 5.5.

In Remark 5.6, we have seen that the panel clustering algorithm is applied on pairs of clusters $(c, s)$ such that for all $(x, y) \in \Gamma_c \times \Gamma_s$, we have

$$|d-n| \leqslant \lambda\sqrt{n} \quad \text{with } d = \|x-y\|/\Delta t \ \text{ and } \ \lambda \text{ as in (5.9)}. \tag{6.1}$$

Hence, we will investigate the function $\omega_n(d)$ only for values of $d$ which satisfy (6.1).

The estimates are obtained in several steps. In the first step, we consider the auxiliary functions

$$\tilde{\omega}_n(d) := 4\pi d\,\Delta t \omega_n^{\Delta t}(d\,\Delta t) = \frac{1}{n!}\left(\frac{d}{2}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{3d}{2}} H_n(\sqrt{2d}), \tag{6.2}$$

which are independent of $\Delta t$. We will determine bounds for the derivatives of $\tilde{\omega}_n(d)$ with respect to $d$ in Theorem 6.5.

Using the Leibniz rule, the derivatives of the original convolution coefficients $\omega_n^{\Delta t}(d)$ with respect to $d$ are given by

$$\partial_d^q \omega_n^{\Delta t}(d) = \frac{1}{4\pi d}\frac{q!}{\Delta t^q}\sum_{l=0}^{q}\frac{1}{l!}\left(-\frac{d}{\Delta t}\right)^{l-q}\tilde{\omega}_n^{(l)}\left(\frac{d}{\Delta t}\right),$$

where $\tilde{\omega}_n^{(l)}(\cdot)$ denotes the $l$th derivative. In the final step, estimates for $\partial_{x_i}^q \omega_n^{\Delta t}(\|x-y\|)$ are obtained in Theorem 6.6.

To find estimates for $\tilde{\omega}_n^{(l)}(d)$, we first consider the functions and their first derivatives. For this, we use an approximation for the Hermite polynomials given by Olver (1963). The proof of the following lemma is given in the extended version of this paper (see Kress & Sauter, 2006, Appendix).

Note that in this paper, $C$ denotes a generic constant independent of $n$, $\Delta t$ and $h$ with, possibly, different values for each inequality.

LEMMA 6.1 The following estimates are valid for $x \geqslant 0$ and $n \geqslant 1$:

$$\left|\mathrm{e}^{-\frac{x^2}{2}} H_n(x)\right| \leqslant Cn!\,\mathrm{e}^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{3}} \tag{6.3}$$

and

$$\left|\partial_x\left(\mathrm{e}^{-\frac{x^2}{2}} H_n(x)\right)\right| \leqslant Cn!\,\mathrm{e}^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{6}} \max\left\{|x^2-(2n+1)|^{\frac{1}{4}} n^{-\frac{1}{12}}, x^{\frac{5}{12}} n^{-\frac{29}{24}}, 1\right\}. \tag{6.4}$$

With Lemma 6.1, we obtain the following estimate for $\tilde{\omega}_n(d)$ and $\tilde{\omega}_n'(d)$.

LEMMA 6.2 For $\tilde{\omega}_n(d)$ as defined in (6.2), the following bound holds for $n \geqslant 1$:

$$|\tilde{\omega}_n(d)| \leqslant Cn^{-\frac{1}{3}} \left(\frac{d}{n}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d-n}{2}} \leqslant Cn^{-\frac{1}{3}}. \tag{6.5}$$

For $n \geqslant 2$ and $|d-n| \leqslant \lambda\sqrt{n}$,

$$|\tilde{\omega}_n'(d)| \leqslant C\lambda n^{-\frac{5}{8}} \left(\frac{d}{n}\right)^{\frac{n}{2}-1} \mathrm{e}^{\frac{d-n}{2}} \leqslant C\lambda n^{-\frac{5}{8}} \tag{6.6}$$

with $\lambda$ as in (5.9).

*Proof.* Due to (6.3), we have

$$|\tilde{\omega}_n(d)| = \frac{1}{n!}\left(\frac{d}{2}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d}{2}} |\mathrm{e}^{-d} H_n(\sqrt{2d})| \leqslant Cn^{-\frac{1}{3}} \left(\frac{d}{n}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d-n}{2}}.$$

The last inequality in (6.5) follows from a straightforward analysis which shows that the maximum of $\left(\frac{d}{n}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d-n}{2}}$ is taken at $n = d$ and hence

$$\left(\frac{d}{n}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d-n}{2}} \leqslant 1. \tag{6.7}$$

For the first derivative, we have

$$\begin{aligned}
\tilde{\omega}_n'(d) &= \frac{1}{n!}\left(\left(\frac{d}{2}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d}{2}} \partial_d(\mathrm{e}^{-d} H_n(\sqrt{2d})) + \partial_d\left(\left(\frac{d}{2}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d}{2}}\right)\mathrm{e}^{-d} H_n(\sqrt{2d})\right) \\
&= \frac{1}{n!}\left(\frac{d}{2}\right)^{\frac{n}{2}} \mathrm{e}^{-\frac{d}{2}} \partial_x \left(\mathrm{e}^{-\frac{x^2}{2}} H_n(x)\right)\Bigg|_{x=\sqrt{2d}} (2d)^{-\frac{1}{2}} - \frac{1}{2}\left(\frac{d}{n}\right)^{-1}\left(\frac{d}{n} - 1\right)\tilde{\omega}_n(d).
\end{aligned}$$

With (6.4) and $|d-n| \leqslant \lambda\sqrt{n}$, we obtain

$$\begin{aligned}
|\tilde{\omega}_n'(d)| &\leqslant C\left(\frac{d}{n}\right)^{\frac{n}{2}-\frac{1}{2}} \mathrm{e}^{-\frac{d-n}{2}} n^{-\frac{2}{3}} \max\left\{\left|d - \left(n + \frac{1}{2}\right)\right|^{\frac{1}{4}} n^{-\frac{1}{12}}, d^{\frac{5}{24}} n^{-\frac{29}{24}}, 1\right\} \\
&\quad + C\lambda n^{-\frac{5}{6}} \left(\frac{d}{n}\right)^{\frac{n}{2}-1} \mathrm{e}^{-\frac{d-n}{2}} \\
&\leqslant C\lambda^{1/4}\left(\frac{d}{n}\right)^{\frac{n}{2}-\frac{1}{2}} \mathrm{e}^{-\frac{d-n}{2}} n^{-\frac{2}{3}} n^{\frac{1}{24}} + C\lambda n^{-\frac{5}{6}}\left(\frac{d}{n}\right)^{\frac{n}{2}-1} \mathrm{e}^{-\frac{d-n}{2}}.
\end{aligned}$$

Finally, with (4.5),

$$\left(\frac{d}{n}\right)^{\frac{1}{2}} \leqslant \left(1 + \frac{|d-n|}{n}\right)^{\frac{1}{2}} \leqslant \left(1 + \frac{\lambda}{\sqrt{n}}\right)^{\frac{1}{2}} \leqslant \left(1 + C\frac{1+\log n}{\sqrt{n}}\right)^{\frac{1}{2}} \leqslant C$$

and by using (6.7), we arrive at (6.6). □

To obtain estimates for the higher derivatives of $\tilde{\omega}_n(d)$, we use the following two lemmas.

LEMMA 6.3 For $n \in \mathbb{N}_0$, the following relation holds:

$$\tilde{\omega}_n'(d) = -\frac{3}{2}\tilde{\omega}_n(d) + 2\tilde{\omega}_{n-1}(d) - \frac{1}{2}\tilde{\omega}_{n-2}(d), \tag{6.8}$$

where formally $\tilde{\omega}_{-1} := \tilde{\omega}_{-2} := 0$.

*Proof.* We recall

$$\hat{k}\left(d, \frac{\gamma(\zeta)}{\Delta t}\right) = \frac{\mathrm{e}^{-\frac{\gamma(\zeta)d}{\Delta t}}}{4\pi d} = \sum_{n=0}^{\infty} \omega_n^{\Delta t}(d)\zeta^n.$$

Using the definition of $\tilde{\omega}_n(d)$, we obtain

$$\mathrm{e}^{-\gamma(\zeta)d} = \sum_{n=0}^{\infty} \tilde{\omega}_n(d)\zeta^n. \tag{6.9}$$

Differentiating both sides of (6.9) with respect to $d$, we obtain

$$-\gamma(\zeta)\mathrm{e}^{-\gamma(\zeta)d} = -\sum_{n=0}^{\infty} \tilde{\omega}_n(d)\gamma(\zeta)\zeta^n = \sum_{n=0}^{\infty} \tilde{\omega}_n'(d)\zeta^n.$$

The statement of the lemma now follows by equating the powers of $\zeta$. □

The following lemma can be obtained from the recursion formula for the Hermite polynomials defined by $H_0(x) = 1$, $H_1(x) = 2x$ and for $n \geqslant 1$,

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

LEMMA 6.4 For $n \in \mathbb{N}_{\geqslant 1}$, the recursion

$$\tilde{\omega}_n(d) = \frac{d}{n}(2\tilde{\omega}_{n-1}(d) - \tilde{\omega}_{n-2}(d)) \tag{6.10}$$

holds.

Now, we can prove a bound for the derivatives of $\tilde{\omega}_n(d)$.

THEOREM 6.5 Let $\frac{n}{2} \geqslant q$, $n \geqslant 1$, and $|d - n| \leqslant \lambda\sqrt{n}$ with $\lambda$ as in (5.9). Then,

$$|\tilde{\omega}_n^{(q)}(d)| \leqslant q!(C\lambda)^q n^{-a_q} \left(\frac{d}{n}\right)^{\frac{n}{2}-q} \mathrm{e}^{-\frac{d-n}{2}} \leqslant q!(C\lambda)^q n^{-a_q}, \tag{6.11}$$

with

$$a_0 = \frac{1}{3}, \quad a_1 = \frac{5}{8} \quad \text{and} \quad a_q = \begin{cases} a_1 + \frac{q-1}{4}, & q \text{ odd}, \\ a_0 + \frac{q}{4}, & q \text{ even}, \end{cases} \tag{6.12}$$

and a generic constant $C$.

*Proof.* The proof is done by induction. For $q = 0$ and $q = 1$, the statement follows from Lemma 6.2.

Next, we show the statement for $q = 2$. For simplicity, we omit the argument $d$ in $\tilde{\omega}_n(d)$ and $\tilde{\omega}'_n(d)$. When differentiating (6.8), we obtain (recall $\tilde{\omega}_{-1} = \tilde{\omega}_{-2} = 0$)

$$\tilde{\omega}''_n = -\frac{3}{2}(\tilde{\omega}'_n - \tilde{\omega}'_{n-1}) + \frac{1}{2}(\tilde{\omega}'_{n-1} - \tilde{\omega}'_{n-2}). \tag{6.13}$$

Using (6.8) and (6.10), we obtain (recall $n \geqslant 1$)

$$\begin{aligned}
\tilde{\omega}'_n &= -\frac{3}{2}\tilde{\omega}_n + 2\tilde{\omega}_{n-1} - \frac{1}{2}\tilde{\omega}_{n-2} \\
&= -\frac{3}{2}\tilde{\omega}_n + \frac{n-1}{2n}\tilde{\omega}_{n-1} + \frac{1}{2n}\tilde{\omega}_{n-1} + \frac{3}{2}\tilde{\omega}_{n-1} - \frac{1}{2}\tilde{\omega}_{n-2} \\
&= \frac{d}{n}\left(-3\tilde{\omega}_{n-1} + \frac{5}{2}\tilde{\omega}_{n-2} - \frac{1}{2}\tilde{\omega}_{n-3}\right) + \frac{1}{2n}\tilde{\omega}_{n-1} + \frac{3}{2}\tilde{\omega}_{n-1} - \frac{1}{2}\tilde{\omega}_{n-2} \\
&= \frac{d}{n}\left(\tilde{\omega}'_{n-1} - \frac{3}{2}\tilde{\omega}_{n-1} + \frac{1}{2}\tilde{\omega}_{n-2}\right) + \frac{1}{2n}\tilde{\omega}_{n-1} + \frac{3}{2}\tilde{\omega}_{n-1} - \frac{1}{2}\tilde{\omega}_{n-2} \\
&= \frac{d}{n}\tilde{\omega}'_{n-1} - \frac{3}{2}\left(\frac{d}{n} - 1\right)\tilde{\omega}_{n-1} + \frac{1}{2}\left(\frac{d}{n} - 1\right)\tilde{\omega}_{n-2} + \frac{1}{2n}\tilde{\omega}_{n-1}.
\end{aligned}$$

Thus,

$$\begin{aligned}
\tilde{\omega}'_n - \tilde{\omega}'_{n-1} &= \left(\frac{d}{n} - 1\right)\left(\tilde{\omega}'_{n-1} - \frac{3}{2}\tilde{\omega}_{n-1} + \frac{1}{2}\tilde{\omega}_{n-2}\right) + \frac{1}{2n}\tilde{\omega}_{n-1} \\
&= \left(\frac{d}{n} - 1\right)\left(-3\tilde{\omega}_{n-1} + \frac{5}{2}\tilde{\omega}_{n-2} - \frac{1}{2}\tilde{\omega}_{n-3}\right) + \frac{1}{2n}\tilde{\omega}_{n-1}.
\end{aligned} \tag{6.14}$$

By using $\left|\frac{d}{n} - 1\right| \leqslant \lambda n^{-\frac{1}{2}}$ and Lemma 6.2, we obtain

$$\begin{aligned}
|\tilde{\omega}'_n - \tilde{\omega}'_{n-1}| &\leqslant C\lambda n^{-\frac{1}{2}}(|\tilde{\omega}_{n-1}| + |\tilde{\omega}_{n-2}| + |\tilde{\omega}_{n-3}|) \\
&\leqslant C\lambda n^{-\frac{1}{2}-\frac{1}{3}}\,\mathrm{e}^{-\frac{d-n}{2}}\left(\sum_{k=1}^{\min\{n-1,3\}}\left(\frac{n-k}{n}\right)^{-\frac{1}{3}}\left(\frac{d}{n}\frac{n}{n-k}\right)^{\frac{n-k}{2}}\right).
\end{aligned}$$

Note that, for any $\alpha \geqslant 0$,

$$\max_{k=1,2,3}\sup_{n\geqslant k+1}\left(\frac{n-k}{n}\right)^{-\alpha} = 2^{\alpha} \quad \text{and} \quad \max_{k=1,2,3}\sup_{n\geqslant k+1}\left(\frac{n}{n-k}\right)^{\frac{n-k}{2}} = \mathrm{e}^{3/2} \tag{6.15}$$

and, hence,

$$|\tilde{\omega}_n' - \tilde{\omega}_{n-1}'| \leqslant C\lambda n^{-\frac{1}{2}-\frac{1}{3}}\,\mathrm{e}^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n-3}{2}}.$$

Using (6.13), (6.15) and Lemma 6.2, we obtain

$$|\tilde{\omega}_n''| \leqslant C\lambda n^{-a_2}\,\mathrm{e}^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n}{2}-2} \tag{6.16}$$

with

$$a_2 = a_0 + \frac{1}{2}.$$

For the induction step $q \to q+1$, we assume that (6.11) holds for $q$. To show that (6.11) also holds for $q+1$, we first differentiate (6.8) $q$ times to obtain

$$\tilde{\omega}_n^{(q+1)} = -\frac{3}{2}(\tilde{\omega}_n^{(q)} - \tilde{\omega}_{n-1}^{(q)}) + \frac{1}{2}(\tilde{\omega}_{n-1}^{(q)} - \tilde{\omega}_{n-2}^{(q)}). \tag{6.17}$$

Furthermore, by differentiating (6.14), we get

$$\begin{aligned}\tilde{\omega}_n^{(q)} - \tilde{\omega}_{n-1}^{(q)} &= \frac{q-1}{n}\left(-3\tilde{\omega}_{n-1}^{(q-2)} + \frac{5}{2}\tilde{\omega}_{n-2}^{(q-2)} - \frac{1}{2}\tilde{\omega}_{n-3}^{(q-2)}\right) + \frac{1}{2n}\tilde{\omega}_{n-1}^{(q-1)}\\ &\quad + \left(\frac{d}{n} - 1\right)\left(-3\tilde{\omega}_{n-1}^{(q-1)} + \frac{5}{2}\tilde{\omega}_{n-2}^{(q-1)} - \frac{1}{2}\tilde{\omega}_{n-3}^{(q-1)}\right).\end{aligned} \tag{6.18}$$

Taking into account (6.1) and the induction assumption, we get

$$\begin{aligned}|\tilde{\omega}_n^{(q)} - \tilde{\omega}_{n-1}^{(q)}| &\leqslant c_1\left\{\frac{q-1}{n}(|\tilde{\omega}_{n-1}^{(q-2)}| + |\tilde{\omega}_{n-2}^{(q-2)}| + |\tilde{\omega}_{n-3}^{(q-2)}|)\right.\\ &\quad \left. + \lambda n^{-\frac{1}{2}}(|\tilde{\omega}_{n-1}^{(q-1)}| + |\tilde{\omega}_{n-2}^{(q-1)}| + |\tilde{\omega}_{n-3}^{(q-1)}|)\right\}\\ &\leqslant c_1\left\{\frac{(q-1)!}{n}(C\lambda)^{q-2}\,\mathrm{e}^{-\frac{d-n}{2}}\sum_{k=1}^{\min\{n-1,3\}}(n-k)^{-a_{q-2}}\left(\frac{d}{n-k}\right)^{\frac{n-k}{2}-q+2}\right.\\ &\quad \left. + \lambda n^{-\frac{1}{2}}(q-1)!(C\lambda)^{q-1}\,\mathrm{e}^{-\frac{d-n}{2}}\sum_{k=1}^{\min\{n-1,3\}}(n-k)^{-a_{q-1}}\left(\frac{d}{n-k}\right)^{\frac{n-k}{2}-q+1}\right\}\\ &\overset{(6.15)}{\leqslant} c_1(q+1)!(C\lambda)^q\,\mathrm{e}^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n-3}{2}-q+1}\left\{n^{-a_{q-2}-1} + n^{-a_{q-1}-\frac{1}{2}}\right\}.\end{aligned}$$

Combining the above equation with (6.17) yields

$$|\tilde{\omega}_n^{(q+1)}| \leqslant (q+1)!(C\lambda)^{q+1}\,\mathrm{e}^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n}{2}-(q+1)} n^{-a_{q+1}}$$

with

$$a_q = \min\left\{a_{q-2} + \frac{1}{2}, a_{q-3} + 1\right\} = \begin{cases} a_1 + \frac{q-1}{4}, & q \text{ odd}, \\ a_0 + \frac{q}{4}, & q \text{ even}. \end{cases}$$

□

We have computed the maximum of the derivatives in numerical experiments to verify the sharpness of estimate (6.11). The results are shown in Table 3. We compare the derivatives of $\tilde{\omega}_{400}(d)$ and $\tilde{\omega}_{600}(d)$ with respect to $d$ and give $\tilde{a}_q = -\log\left(\frac{\|\tilde{\omega}_{400}^{(q)}(d)\|_\infty}{\|\tilde{\omega}_{600}^{(q)}(d)\|_\infty}\right)\Big/ \log(2/3)$. It can be seen that $\tilde{a}_q \approx 0.33 + 0.3q$, i.e. $b \approx 0.3$ which compares well with the theoretical result $b \geqslant 0.25$.

From the bounds on the derivatives of $\tilde{\omega}_n(d)$, we now obtain estimates for $\left|\partial_{x_i}^q \omega_n^{\Delta t}(\|x-y\|)\right|$.

THEOREM 6.6 For $\frac{n}{2} \geqslant q$ and $\left|\frac{\|x-y\|}{\Delta t} - n\right| \leqslant \lambda\sqrt{n}$ with $\lambda$ as in (5.9), we have

$$\begin{aligned} \left|\partial_{x_i}^q \omega_n^{\Delta t}(\|x-y\|)\right| &\leqslant \frac{(C\lambda)^q q!}{4\pi\|x-y\|} \Delta t^{-q} n^{-a_q} \left(\frac{\|x-y\|}{n\Delta t}\right)^{\frac{n}{2}-q} \mathrm{e}^{-\frac{\frac{\|x-y\|}{\Delta t}-n}{2}} \\ &\leqslant \frac{(C\lambda)^q q!}{\|x-y\|} \Delta t^{-q} n^{-a_q}, \end{aligned}$$

where $C > 0$ is a generic constant independent of the discretization parameters.

For the proof of Theorem 6.6, we need the following lemma.

LEMMA 6.7 Let $d = d(x,y) = \sqrt{\sum_{i=1}^3 (x_i - y_i)^2}$. For a function $f(d)$, we have for $q \geqslant 1$,

$$\left|\partial_{x_i}^q f(d)\right| \leqslant C^q q! \max_{1\leqslant \nu\leqslant q} \frac{1}{\nu!} |f^{(\nu)}(d)| \frac{1}{d^{q-\nu}}.$$

*Proof.* By induction, one can easily prove that

$$\partial_{x_i}^q f(d) = \sum_{\nu=1}^{q} g_{\nu,q}(x,y) f^{(\nu)}(d),$$

with $g_{1,1}(x,y) = \frac{x_i - y_i}{d}$ and for $q \geqslant 2$ and $1 \leqslant \nu \leqslant q$,

$$g_{\nu,q}(x,y) = \partial_{x_i} g_{\nu,q-1}(x,y) + g_{\nu-1,q-1}(x,y)\frac{x_i - y_i}{d},$$

with $g_{0,q} = g_{q,q-1} = 0$. In addition, we show by induction that

$$g_{\nu,q}(x,y) = \sum_{\mu=0}^{\min\left\{\left\lfloor \frac{q}{2}\right\rfloor, q-\nu\right\}} \alpha_{\mu,\nu}^q \frac{(x_i - y_i)^{q-2\mu}}{d^{2q-\nu-2\mu}}, \quad 1 \leqslant \nu \leqslant q, \tag{6.19}$$

TABLE 3 *$\tilde{a}_q$ for $0 \leqslant q \leqslant 6$*

| $q$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|---|
| | 0.33 | 0.63 | 0.92 | 1.24 | 1.50 | 1.82 | 2.13 |

for some coefficients $\alpha^q_{\mu,\nu}$. For $q = 1$, the statement follows from the definition of $g_{1,1}(x, y)$ with $a^1_{0,1} = 1$.

Assume that (6.19) holds for some $q$. Then,

$$
\begin{aligned}
g_{\nu,q+1}(x,y) &= \partial_{x_i} g_{\nu,q}(x,y) + g_{\nu-1,q}(x,y)\frac{x_i - y_i}{d} \\
&= \sum_{\mu=0}^{\min\left\{\left\lfloor \frac{q}{2}\right\rfloor, q-\nu\right\}} (q-2\mu)\alpha^q_{\mu,\nu}\frac{(x_i-y_i)^{q-2\mu-1}}{d^{2q-\nu-2\mu}} \\
&\quad - \sum_{\mu=0}^{\min\left\{\left\lfloor \frac{q}{2}\right\rfloor, q-\nu\right\}} (2q-\nu-2\mu)\alpha^q_{\mu,\nu}\frac{(x_i-y_i)^{q+1-2\mu}}{d^{2q+2-\nu-2\mu}} \\
&\quad + \sum_{\mu=0}^{\min\left\{\left\lfloor \frac{q}{2}\right\rfloor, q-\nu\right\}} \alpha^q_{\mu,\nu-1}\frac{(x_i-y_i)^{q-2\mu+1}}{d^{2q-\nu+2-2\mu}} \\
&= \sum_{\mu=0}^{\min\left\{\left\lfloor \frac{q+1}{2}\right\rfloor, q+1-\nu\right\}} \alpha^{q+1}_{\mu\nu}\frac{(x_i-y_i)^{(q+1)-2\mu}}{d^{2(q+1)-\nu-2\mu}}
\end{aligned}
$$

with

$$
\alpha^{q+1}_{\mu,\nu} = (q-2(\mu-1))\alpha^q_{\mu-1,\nu} - (2q-\nu-2\mu)\alpha^q_{\mu,\nu} + \alpha^q_{\mu,\nu-1}, \tag{6.20}
$$

where we set all coefficients $\alpha^q_{\mu,\nu}$ not occurring in (6.19) to 0. Thus,

We show by induction that $|\alpha^q_{\mu,\nu}| \leqslant c_1^q \frac{(q-1)!}{\nu!}$ for some constant $c_1$. First, for $q = 1$, we have $\alpha^1_{0,1} = 1$.

Let $|\alpha^q_{\mu,\nu}| \leqslant c_1^q \frac{(q-1)!}{\nu!}$ for some $q$. We use (6.20) and $\nu \leqslant q + 1$ to obtain

$$
|\alpha^{q+1}_{\mu,\nu}| \leqslant 3qc_1^q\frac{(q-1)!}{\nu!} + c_1^q\nu\frac{(q-1)!}{\nu!} \leqslant c_1^{q+1}\frac{q!}{\nu!},
$$

when choosing $c_1$ large enough. Combining the above equation with (6.19) results in

$$
|g_{\nu,q}(x,y)| \leqslant c_1^q\frac{q!}{\nu!}\frac{1}{d^{q-\nu}}.
$$

Using $q \leqslant 2^q$, we obtain

$$
\begin{aligned}
\left|\partial^q_{x_i} f(d)\right| &\leqslant q \max_{1\leqslant\nu\leqslant q} |g_{\nu,q}(x,y)||f^{(\nu)}(d)| \\
&\leqslant (2c_1)^q q! \max_{1\leqslant\nu\leqslant q}\frac{1}{\nu!}|f^{(\nu)}(d)|\frac{1}{d^{q-\nu}}.
\end{aligned}
$$

□

*Proof of Theorem* 6.6. For simpler notation, we write $d = \|x - y\|$. We have

$$\omega_n^{\Delta t}(d) = \frac{1}{4\pi d}\tilde{\omega}_n\left(\frac{d}{\Delta t}\right)$$

and

$$\partial_d^q \omega_n^{\Delta t}(d) = \frac{1}{4\pi d}\frac{1}{\Delta t^q}\sum_{l=0}^{q}\frac{q!}{l!}\left(-\frac{d}{\Delta t}\right)^{l-q}\tilde{\omega}_n^{(l)}\left(\frac{d}{\Delta t}\right) \tag{6.21}$$

For $q = 0$, the statement of the theorem follows easily by combining (6.5) with (6.21). For $q \geqslant 1$, from Theorem 6.5 and Lemma 6.7, we conclude that (recall $n/2 \geqslant q$)

$$\begin{aligned}
\left|\partial_{x_i}^q \omega_n^{\Delta t}(d)\right| &\leqslant C^q q! \max_{1\leqslant\nu\leqslant q}\frac{1}{\nu!}|\partial_d^\nu \omega_n^{\Delta t}(d)| d^{-q+\nu}\\
&\leqslant \frac{C^q q!}{4\pi d}\max_{1\leqslant\nu\leqslant q}\frac{1}{\Delta t^\nu}\sum_{l=0}^{\nu}\frac{1}{l!}\left(\frac{d}{\Delta t}\right)^{l-\nu} d^{-q+\nu}\left|\tilde{\omega}_n^{(l)}\left(\frac{d}{\Delta t}\right)\right|\\
&\leqslant \frac{C^q q!}{4\pi d}\max_{1\leqslant\nu\leqslant q}\sum_{l=0}^{\nu}(C\lambda)^l d^{l-q} n^{-a_l}\Delta t^{-l}\left(\frac{d}{n\Delta t}\right)^{\frac{n}{2}-l}\mathrm{e}^{-\frac{\frac{d}{\Delta t}-n}{2}}\\
&= \frac{C^q q!}{4\pi d}\Delta t^{-q}\left(\frac{d}{n\Delta t}\right)^{\frac{n}{2}-q}\mathrm{e}^{-\frac{\frac{d}{\Delta t}-n}{2}}\max_{1\leqslant\nu\leqslant q}\sum_{l=0}^{\nu}(C\lambda)^l n^{-a_l-q+l}.
\end{aligned}$$

From (6.12), it is easy to see

$$a_q - a_l - q + l \leqslant 0$$

and, hence,

$$\left|\partial_{x_i}^q \omega_n^{\Delta t}(d)\right| \leqslant \frac{C^q q!}{4\pi d}\Delta t^{-q}\left(\frac{d}{n\Delta t}\right)^{\frac{n}{2}-q}\mathrm{e}^{-\frac{\frac{d}{\Delta t}-n}{2}} n^{-a_q}\frac{(C\lambda)^{q+1}-1}{C\lambda - 1},$$

where as before $C$ denotes a generic constant. The last term is bounded by $2(C\lambda)^q$ provided $C\lambda \geqslant 2$. □

TABLE 4 *Storage requirements for sparse approximation: $n = 0$ and $\Delta t = 0.1$*

| $M$ | $\mathbf{A}_{\text{full}}$ | $\mathbf{A}_{\text{sparse}}$ | Relative error |
|---|---|---|---|
| 8192 | 512 MB | 4.4 MB | $7.1 \times 10^{-3}$ |
| | | 16.2 MB | $7.3 \times 10^{-4}$ |
| | | 34 MB | $8.2 \times 10^{-5}$ |
| | | 63.1 MB | $5.0 \times 10^{-6}$ |
| | | 91.5 MB | $6.2 \times 10^{-7}$ |
| | | 124 MB | $7.7 \times 10^{-8}$ |

TABLE 5 *Storage requirements for panel clustering approximation: $n = 15$ and $\Delta t = 0.2$*

| $M$ | $\mathbf{A}_{\text{full}}$ | $q$ | $\mathbf{A}_{\text{pc}}$ | Relative error |
|---|---|---|---|---|
| 32768 | 8192 MB | 3 | 22.6 MB | $2.0 \times 10^{-3}$ |
| | | 4 | 139 MB | $8.0 \times 10^{-4}$ |

TABLE 6 *Storage requirements for panel clustering approximation: $n = 30$ and $\Delta t = 0.1$*

| $M$ | $\mathbf{A}_{\text{full}}$ | $q$ | $\mathbf{A}_{\text{pc}}$ | Relative error |
|---|---|---|---|---|
| 32768 | 8192 MB | 3 | 22.6 MB | $5.0 \times 10^{-2}$ |
| | | 4 | 139 MB | $1.7 \times 10^{-2}$ |

## 7. Outlook

In this paper, we have analysed a panel clustering approximation for the wave equation. We have derived upper bounds for both storage requirements and computational complexity. From the theoretical point of view, the cut off and panel clustering approximation results in a significant reduction of the complexity. However, in a next step, it is important to perform numerical experiments to see at what problem size the asymptotic gain of our method becomes dominant.

In Tables 4–6, we show the results of some preliminary numerical tests to illustrate the storage gain. In Table 4, we have considered $n = 0$ and the sparse approximation technique only. In Tables 5 and 6, we have considered the panel clustering approach for two different $n$ and $\Delta t$.

Additional tests have shown that a recompression technique based on a singular value decomposition of the blocks and possibly joining of several blocks (Grasedyck, 2004) leads to much reduced storage requirements especially for increasing $q$.

We have not yet addressed the need of special quadrature techniques. One benefit of the panel clustering technique is the fact that no integration of the kernel functions is necessary. The only integrals required involve Lagrange polynomials and the basis functions of the boundary element space. For the cut off approximation, we still need to integrate the kernel functions $\omega_n^{\Delta t}$. For the efficient computation of these integrals, the choice of the quadrature method is important.

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