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Numerical Treatment of Retarded Boundary Integral Equations by Sparse Panel Clustering (extended version)
(revised version: June 2007)
by

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# Numerical treatment of Retarded Boundary Integral Equations by Sparse Panel Clustering (extended version) 

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#### Abstract

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 cutoff, 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.


## 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 [11]). 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 three dimensional problem and denote by $h$ a typical meshsize in the spatial discretization, the boundary integral equation leads to $\mathcal{O}\left(h^{-2}\right)$ unknowns instead of $\mathcal{O}\left(h^{-3}\right)$, 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

[^0]complexity. For potential problems of elliptic type, fast methods (panel clustering, wavelets, multipole, $\mathcal{H}$-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 [21], [23]. In [16], [17], we have introduced two advanced versions of the method in order to reduce its complexity. In [16], a sparse approximation technique has been developed, where a simple cutoff 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 [16]. 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 discretisation methods which include collocation methods with some stabilization techniques (cf. [3], [4], [6], [7], [8], [24], [26]) and Laplace-Fourier methods coupled with Galerkin boundary elements in space ([1], [5], [9], [14]). Numerical experiments can be found, e.g., in [15].

In [10] a fast version of the marching-on-in-time (MOT) 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 [20, 29]. A related, interesting variation of the convolution quadrature for convolution kernels whose Laplace transform is sectorial can be found in [28].

Another method which is also based on the convolution quadrature is presented in [2], 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 three dimensional 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

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

To formulate the problem as a boundary integral equation, $u(x, t)$ can be written as a single layer potential

$$
u(x, t)=\int_{0}^{t} \int_{\Gamma} \frac{\delta(t-\tau-\|x-y\|}{4 \pi\|x-y\|} \phi(y, \tau) d s_{y} d \tau
$$

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

$$
\begin{equation*}
\int_{0}^{t} \int_{\Gamma} k(\|x-y\|, t-\tau) \phi(y, \tau) d s_{y} d \tau=g(x, t) \quad \forall(x, t) \in \Gamma \times(0, T) \tag{1}
\end{equation*}
$$

with the kernel function

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

## 3 Convolution Quadrature Method

A time discretization of (1) can be obtained by introducing a stepsize $\Delta t$ and a maximal number of time steps $N$, and replacing the time convolution in (1) at time step $t_{n}=n \Delta t$ by a discrete convolution,

$$
\begin{equation*}
\sum_{j=0}^{n} \int_{\Gamma} \omega_{n-j}^{\Delta t}(\|x-y\|) \phi\left(y, t_{j}\right) d s_{y}=g\left(x, t_{n}\right) \quad \forall x \in \Gamma, 1 \leq n \leq N \tag{2}
\end{equation*}
$$

with convolution weights $\omega_{n}^{\Delta t}(d)$.
We use the convolution quadrature method [21], [23], to obtain 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 [16], [17], [23]. We here only give the definition of the quadrature weights.

Definition 1. Let

$$
\begin{equation*}
\sum_{j=0}^{k} \alpha_{j} u^{n+j-k}=\Delta t \sum_{j=0}^{k} \beta_{j} f\left(u^{n+j-k}\right) \tag{3}
\end{equation*}
$$

be a linear multistep method for an ordinary differential equation $u^{\prime}(t)=f(u(t))$, where $u^{n} \approx$ $u\left(t_{n}\right)$. 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 2. Given a linear multistep method (3), 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 $\hat{k}(d, s):=\frac{e^{-s d}}{4 \pi d}$ is the Laplace transform of the kernel function $k(d, t)=\frac{\delta(t-d)}{4 \pi d}$ in (1).

The convolution weights can be derived by Taylor expansion,

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

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

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

In that case, using the formula for multiple differentiation of composite functions (see, e.g., [12]), we obtain the explicit representation

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

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) is A-stable and second order accurate, then so is (2). Stability and convergence results for the semi discrete problem can be found in [16] and [23].

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 $\left(b_{i}(x)\right)_{i=1}^{M}$. For the Galerkin boundary element method, we replace $\phi\left(y, t_{j}\right)$ in (2) by

$$
\phi_{\Delta t, h}^{j}(y)=\sum_{i=1}^{M} \phi_{j, i} b_{i}(y)
$$

and impose the integral equation in a weak form

$$
\sum_{j=0}^{n} \sum_{i=1}^{M} \phi_{j, i} \int_{\Gamma} \int_{\Gamma} \omega_{n-j}^{\Delta t}(x-y) b_{i}(y) b_{k}(x) d s_{y} d s_{x}=\int_{\Gamma} g\left(x, t_{n}\right) b_{k}(x) d s_{x}
$$

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

$$
\begin{equation*}
\sum_{j=0}^{n} \mathbf{A}_{n-j} \phi_{j}=\mathbf{g}_{n}, \quad n=1, \ldots, N \tag{4}
\end{equation*}
$$

with

$$
\left(\mathbf{A}_{n-j}\right)_{k, i}:=\int_{\Gamma} \int_{\Gamma} \omega_{n-j}^{\Delta t}(x-y) b_{i}(y) b_{k}(x) d s_{y} d s_{x}
$$

and

$$
\left(\mathbf{g}_{n}\right)_{k}=\int_{\Gamma} g(x, n \Delta t) b_{k}(x) d s_{x}
$$

The compact formulation as a block triangular system is given by

$$
\begin{equation*}
\overrightarrow{\mathbf{A}}_{N} \vec{\phi}_{N}=\overrightarrow{\mathbf{g}}_{N} \tag{5}
\end{equation*}
$$

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

$$
\overrightarrow{\mathbf{A}}_{N}:=\left(\begin{array}{cccccc}
\mathbf{A}_{0} & \mathbf{0} & \ldots & & & \mathbf{0}  \tag{6}\\
\mathbf{A}_{1} & \mathbf{A}_{0} & \ddots & & & \vdots \\
\mathbf{A}_{2} & \mathbf{A}_{1} & \ddots & & & \\
\vdots & \mathbf{A}_{2} & \ddots & & \ddots & \\
& & \ddots & \ddots & \ddots & \mathbf{0} \\
\mathbf{A}_{N} & \ldots & & \mathbf{A}_{2} & \mathbf{A}_{1} & \mathbf{A}_{0}
\end{array}\right) \quad \text { and } \quad \overrightarrow{\mathbf{g}}_{N}:=\left(\begin{array}{c}
\mathbf{g}_{0} \\
\mathbf{g}_{1} \\
\vdots \\
\mathbf{g}_{N}
\end{array}\right)
$$

The matrices $\mathbf{A}_{j}$ have dimension $M \times M$ and are fully populated. The following simple procedure is the algorithmic formulation of (5).

## procedure solve;

begin
for $i:=0$ to $N$ do begin
$\mathrm{s}:=\mathrm{g}_{i}$;
for $j:=0$ to $i-1$ do

$$
\begin{equation*}
\mathbf{s}:=\mathbf{s}-\mathbf{A}_{i-j} \phi_{j} \tag{7}
\end{equation*}
$$

solve

$$
\begin{equation*}
\mathbf{A}_{0} \phi_{i}=\mathbf{s} \tag{8}
\end{equation*}
$$

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 Cutoff

The matrices in (4) are densely populated. This is due to the fact that, although the basis functions have local support, they are coupled by the nonlocal convolution coefficients $\omega_{n}^{\Delta t}(d)$. In [16], 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 nonlocal functions, they can be replaced by more localized functions. In Figure 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 $\mathcal{O}(\Delta t \sqrt{n})$, they are small enough to be replaced by 0 . In [16], the following results are shown.



Figure 1: Convolution weight $\omega_{n}^{\Delta t}(d), n=100, n=200, \Delta t=1$.

Lemma 3. Let

$$
I_{n, \varepsilon}^{\Delta t}:= \begin{cases}{\left[0, \frac{2}{3} \Delta t|\log \varepsilon|\right],} & n=0,  \tag{9}\\ {\left[t_{n}-3 \Delta t \sqrt{n}|\log \varepsilon|, t_{n}+3 \Delta t \sqrt{n}|\log \varepsilon|\right] \cap \operatorname{diam}(\Omega),} & n>0 .\end{cases}
$$

Then there holds

$$
\begin{equation*}
\left|\omega_{n}^{\Delta t}(d)\right| \leq \frac{\varepsilon}{4 \pi d} \quad \forall d \notin I_{n, \varepsilon}^{\Delta t} . \tag{10}
\end{equation*}
$$

Replacing $\omega_{n}^{\Delta t}(d)$ by zero outside the interval $I_{n, \varepsilon}^{\Delta t}$ leads to the following sparse approximation.
Definition 4. For a given error tolerance $\varepsilon$, let

$$
\mathcal{P}_{\varepsilon, n}:=\left\{(i, j) \mid \exists(x, y) \in \operatorname{supp} b_{i} \cap \operatorname{supp} b_{j}:\|x-y\| \in I_{n, \varepsilon}^{\Delta t}\right\} .
$$

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

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

The solutions of the algebraic system

$$
\begin{equation*}
\sum_{j=0}^{n} \tilde{\mathbf{A}}_{n-j} \tilde{\phi}_{j}=\mathbf{g}_{n}, \quad n=1, \ldots, N \tag{11}
\end{equation*}
$$

are the coefficient vectors of the approximate Galerkin solutions

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

The following theorem follows directly from [16, Theorem 4.7] by using $\frac{1-e^{-\sigma \Delta t}}{2 c_{\Delta c_{\sigma}}} \leq C \Delta t$ therein.
Theorem 5. 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 $0<\varepsilon<C h \Delta t^{3}$, the approximate Galerkin solutions $\tilde{\phi}_{\Delta t, h}^{n}$ exist and satisfy the error estimate

$$
\begin{equation*}
\left\|\tilde{\phi}_{\Delta t, h}^{n}-\phi(\cdot, t)\right\|_{H^{-1 / 2}(\Gamma)} \leq C_{g}(T)\left(\varepsilon h^{-1} \Delta t^{-5}+\Delta t^{2}+h^{m+3 / 2}\right) \tag{12}
\end{equation*}
$$

Remark 6. The choice

$$
\begin{equation*}
\Delta t^{2} \sim h^{m+3 / 2} \quad \text { and } \quad \varepsilon \sim(\Delta t)^{7} h \sim h^{7 m / 2+25 / 4} \tag{13}
\end{equation*}
$$

balances the three error terms in (12).

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

$$
\begin{equation*}
\mathcal{O}\left(M \max \left\{1, t_{n}^{\frac{3}{2}} \sqrt{\Delta t} M \log M\right\}\right) \tag{14}
\end{equation*}
$$

and some cases are summarized in Table 4, assuming that $\Delta t^{2} \sim h^{m+\frac{3}{2}}$. The total storage amount follows by summing (14) for $n=0,1, \ldots, N$. By using $(N \Delta t)^{2} \sim 1$ and $M \geq \mathcal{O}(N)$ we obtain

$$
\text { total storage amount for all } \tilde{\mathbf{A}}_{n}, \quad 0 \leq n \leq N: \quad \mathcal{O}\left(N^{1 / 2} M^{2} \log M\right)
$$

This is a significant reduction of the storage cost by a factor of $\mathcal{O}\left(N^{1 / 2}\right)$ compared to the original Galerkin method where the storage cost is $\mathcal{O}\left(N M^{2}\right)$.
Remark 7. In [19], [21], [22], [23], FFT-techniques have been introduced to solve the system (5). While the storage costs stay unchanged $\mathcal{O}\left(N M^{2}\right)$ the computational complexity is reduced from $\mathcal{O}\left(N^{2} M^{2}\right)$ to $\mathcal{O}\left(N \log ^{2} N M^{2}\right)$. Our cutoff strategy reduces the storage cost to $\mathcal{O}\left(N^{1 / 2} M^{2}\right)$ 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 17.

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

Table 1: Storage requirements for $\tilde{\mathbf{A}}_{n}$

The subroutine procedure solve (cf. Section 3) can easily be modified to take into account the sparse approximation by replacing step (7) by

$$
\begin{equation*}
\text { for all } 1 \leq k \leq M: \quad s_{k}:=s_{k}-\sum_{\ell:(k, \ell) \in \mathcal{P}_{\varepsilon, i-j}}\left(\mathbf{A}_{i-j}\right)_{k, \ell} \phi_{j, \ell} \tag{15}
\end{equation*}
$$

while the iterative solution of (8) should take into account the sparsity of $\tilde{\mathbf{A}}_{0}$ as well.

## 5 Panel Clustering

The panel clustering method was developed in [18] 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, $\mathcal{H}$-matrices etc. exist. However, these fast methods (with the exception of $\mathcal{H}$-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 cutoff strategy as in Section 4, a matrix-vector multiplication $\tilde{\mathbf{A}}_{n} \phi$ with a vector $\phi=\left(\phi_{i}\right)_{i=1}^{M} \in \mathbb{R}^{M}$ can be written in the form

$$
\begin{equation*}
\forall 1 \leq k \leq M: \quad\left(\tilde{\mathbf{A}}_{n} \phi\right)_{k}=\sum_{\ell:(k, \ell) \in \mathcal{P}_{\varepsilon, n}} \phi_{\ell} \int_{\Gamma} \int_{\Gamma} \omega_{n}^{\Delta t}(\|x-y\|) b_{\ell}(y) b_{k}(x) d \Gamma_{y} d \Gamma_{x} . \tag{16}
\end{equation*}
$$

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

$$
\begin{equation*}
n>n^{p c}:=C \max \left\{\log ^{2} M, M^{m-\frac{1}{2}} \log ^{4} M\right\} \tag{17}
\end{equation*}
$$

for some constant $C$. For $n<n^{p c}$, it will turn out that, for the simple cutoff strategy, the complexity has the same asymptotic behaviour. (Note that for the first time steps the simple
cutoff strategy reduces the complexity much more significantly than for the later time steps, see Table 4.)

Let $\mathbb{N}_{M}:=\{1,2, \ldots, M\}$.
Definition 8. A cluster $c$ is a subset of $\mathbb{N}_{M}$. If $c$ is a cluster, the corresponding subdomain of $\Gamma$ is $\Gamma_{c}:=\bigcup_{i \in t} \operatorname{supp}\left(b_{i}\right)$. The cluster box $Q_{c} \subset \mathbb{R}^{3}$ is the minimal axisparallel cuboid which contains $\Gamma_{c}$ and the cluster size $L_{c}$ is the maximal side length of $Q_{c}$.

Definition 9. Let $\varepsilon>0$ and $n>n^{p c}$. 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

$$
\begin{equation*}
\max \left\{L_{c}, L_{s}\right\} \leq \eta \frac{\Delta t n^{b}}{|\log \varepsilon|} \tag{18}
\end{equation*}
$$

The power $b$ in (18) is a fixed number. Some comments are given in Remark 10.
Remark 10. In Section 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 cutoff). 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 (18) satisfies

$$
\begin{equation*}
0.25 \leq b \leq 0.3 \tag{19}
\end{equation*}
$$

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

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

and

$$
\mathcal{P}_{\varepsilon, n} \subset \bigcup_{(c, s) \in \mathcal{P}_{\varepsilon, n}^{\mathrm{Pc}}}(c, s)
$$

We skip here the explicit formulation of the divide-and-conquer algorithm for the efficient construction of $\mathcal{P}_{\varepsilon, n}^{\mathrm{pc}}$ by introducing a tree structure for the clusters but refer, e.g., to [27] for the details.

Expression (16) becomes

$$
\begin{equation*}
\left(\tilde{\mathbf{A}}_{n} \phi\right)_{k}=\sum_{(c, s) \in \mathcal{P}_{\mathcal{E}, n}^{\mathrm{p}}} \sum_{\ell:(k, \ell) \in(c, s)} \phi_{\ell} \int_{\Gamma_{c}} \int_{\Gamma_{s}} \omega_{n}^{\Delta t}(\|x-y\|) b_{\ell}(y) b_{k}(x) d \Gamma_{y} d \Gamma_{x} \tag{20}
\end{equation*}
$$

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 in $Q_{c} \times Q_{s}$ we may define an approximation by Čebyšev interpolation:

$$
\begin{equation*}
\omega_{n}^{\Delta t}(\|x-y\|) \approx \check{\omega}_{n}^{\Delta t}(\|x-y\|)=\sum_{\mu, \nu \in\left(\mathbb{N}_{q}\right)^{3}} \mathcal{L}_{c}^{(\mu)}(x) \mathcal{L}_{s}^{(\nu)}(y) \omega_{n}^{\Delta t}\left(\left\|x^{\mu}-y^{\nu}\right\|\right) \tag{21}
\end{equation*}
$$

where $\mathcal{L}_{c}^{(\mu)}$ and $\mathcal{L}_{s}^{(\nu)}$, resp., are the tensorized versions of the $q$-th order Lagrange polynomials (properly scaled and translated to $Q_{c}$ and $Q_{s}$, resp.) corresponding to the tensorized Čebyšev nodes $x^{\mu}$ and $y^{\nu}$ for $Q_{c}$ and $Q_{s}$, resp. Replacing the kernel functions $\omega_{n}^{\Delta t}$ under the integral in (20) allows to perform the integration with respect to $x$ and $y$ separately. This leads to

$$
\begin{aligned}
& \sum_{\ell:(k, \ell) \in(c, s)} \phi_{\ell} \int_{\Gamma_{c}} \int_{\Gamma_{s}} \omega_{n}^{\Delta t}(\|x-y\|) b_{\ell}(y) b_{k}(x) d \Gamma_{y} d \Gamma_{x} \\
& \approx \sum_{\ell:(k, \ell) \in(c, s)} \sum_{\mu, \nu \in\left(\mathbb{N}_{q}\right)^{3}} \mathbf{V}_{c}^{(\mu, k)} \mathbf{S}_{(c, s)}^{\mu, \nu} \mathbf{V}_{s}^{(\nu, \ell)} \phi_{\ell},
\end{aligned}
$$

where

$$
\begin{equation*}
\mathbf{V}_{c}^{(\mu, k)}:=\int_{\Gamma_{c}} \mathcal{L}_{c}^{(\mu)}(x) b_{k}(x) d \Gamma_{x} \quad \text { and } \quad \mathbf{S}_{(c, s)}^{\mu, \nu}:=\omega_{n}^{\Delta t}\left(\left\|x^{\mu}-y^{\nu}\right\|\right) \tag{22}
\end{equation*}
$$

Hence, the panel clustering approximation of (7) is given by replacing step (7) by

$$
\begin{equation*}
s_{k}:=s_{k}-\sum_{(c, s) \in \mathcal{P}_{\mathcal{P}, n}^{\mathrm{pc}}} \sum_{\ell:(k, \ell) \in(c, s)} \sum_{\mu, \nu \in\left(\mathbb{N}_{q}\right)^{3}} \mathbf{V}_{c}^{(\mu, k)} \mathbf{S}_{(c, s)}^{\mu, \nu} \mathbf{V}_{s}^{(\nu, \ell)} \phi_{\ell} . \tag{23}
\end{equation*}
$$

Remember that for the first time steps, the matrices $\mathbf{A}_{n}$ are approximated using the simple cutoff strategy.

Remark 11. 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 (13))

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

which is always satisfied.
For $m=1$, we get (with $b=1 / 4$ )

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

Hence, the condition

$$
n \geq C M^{1 / 2} \log ^{4} M=\mathcal{O}\left(h^{-1}|\log h|^{4}\right)
$$

ensures $\eta \frac{\Delta t n^{b}}{|\log \varepsilon|} \geq C h$. Note, that this is guaranteed by (17).

Although the admissibility criterion (18) 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., [27] 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

$$
\begin{aligned}
& \sup _{z \in Q_{c}-Q_{s}}\left|\omega_{n}^{\Delta t}(\|z\|)-\check{\omega}_{n}^{\Delta t}(\|z\|)\right| \leq \\
& C \frac{L^{q+1}\left(1+\log ^{5} q\right)}{2^{2 q+1}(q+1)!} \max _{i \in\{1,2,3\}} \sup _{z \in Q_{c}-Q_{s}}\left|\partial_{z_{i}}^{q+1} \omega(\|z\|)\right|,
\end{aligned}
$$

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 $\left\{x-y:(x, y) \in Q_{c} \times Q_{s}\right\}$.
Theorem 12. For $(c, s) \in \mathcal{P}_{\varepsilon, n}^{\mathrm{pc}}$, assume that the partial derivatives of $\omega_{n}^{\Delta t}(\|x-y\|)$ satisfy

$$
\begin{equation*}
\max _{1 \leq i \leq 3}\left|\partial_{z_{i}}^{q} \omega_{n}^{\Delta t}(\|z\|)\right| \left\lvert\, \leq q!\|z\|^{-1}\left(\frac{C \lambda}{\Delta t n^{b}}\right)^{q} \quad \forall z \in Q_{c}-Q_{s} .\right. \tag{12a}
\end{equation*}
$$

Then

$$
\begin{equation*}
\left|\check{\omega}_{n}^{\Delta t}(\|x-y\|)-\omega_{n}^{\Delta t}(\|x-y\|)\right| \leq \frac{C_{1}}{\operatorname{dist}\left(Q_{c}, Q_{s}\right)}\left(\frac{C_{2} \max \left\{L_{c}, L_{s}\right\} \lambda}{\Delta t n^{b}}\right)^{q+1} \tag{12b}
\end{equation*}
$$

The validity of assumption (12a) with $b$ as in Definition 9 and

$$
\begin{equation*}
\lambda:=2 \eta+3|\log \varepsilon| . \tag{24}
\end{equation*}
$$

will be derived in Theorem 23.
Remark 13. Note that the panel clustering is applied on blocks $(c, s) \subset \mathcal{P}_{\varepsilon, n}$ which satisfy (18) and, hence there exists $\left(x_{0}, y_{0}\right) \in \Gamma_{c} \times \Gamma_{s}$ such that

$$
\left|\left\|x_{0}-y_{0}\right\|-t_{n}\right| \leq \tilde{\lambda} \Delta t \sqrt{n} \quad \text { with } \quad \tilde{\lambda}:=3|\log \varepsilon|
$$

As a consequence we have, for any $(x, y) \in \Gamma_{c} \times \Gamma_{s}$, (recall $b<1 / 2$ )

$$
\begin{aligned}
\left|\|x-y\|-t_{n}\right| & \leq\left|\|x-y\|-\left\|x_{0}-y_{0}\right\|\right|+\tilde{\lambda} \Delta t \sqrt{n} \leq L_{c}+L_{s}+\tilde{\lambda} \Delta t \sqrt{n} \\
& \leq\left(2 \eta n^{b-1 / 2}+\tilde{\lambda}\right) \Delta t \sqrt{n} \leq \lambda \Delta t \sqrt{n}
\end{aligned}
$$

with $\lambda$ as in (24).

Theorem 14. Let $0<\varepsilon<\frac{1}{8}$ and $n>16\left|\log ^{2} \varepsilon\right|$. Let the assumptions of Theorem 12 be satisfied and the interpolation order chosen according to $q \geq|\log \varepsilon| / \log 2$. Let $(c, s) \in \mathcal{P}_{\varepsilon, n}^{\mathrm{pc}}$ be admissible for some $0<\eta \leq \eta_{0}$ and sufficiently small $\eta_{0}=\mathcal{O}(1)$. Then

$$
\begin{equation*}
\left|\check{\omega}_{n}^{\Delta t}(\|x-y\|)-\omega_{n}^{\Delta t}(\|x-y\|)\right| \leq C \frac{\varepsilon}{\|x-y\|} \quad \forall(x, y) \in \Gamma_{c} \times \Gamma_{s} \tag{25}
\end{equation*}
$$

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

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

$$
\left|\|x-y\|-t_{n}\right| \leq \frac{\lambda t_{n}}{\sqrt{n}} \quad \forall(x, y) \in \Gamma_{c} \times \Gamma_{s}
$$

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

$$
t_{n} \leq\left(1-\frac{\lambda}{\sqrt{n}}\right)^{-1}\|x-y\|
$$

We also have

$$
\begin{aligned}
\operatorname{dist}\left(Q_{c}, Q_{s}\right) & \geq\|x-y\|-\sqrt{3}\left(L_{c}+L_{s}\right) \geq\|x-y\|-2 \sqrt{3} \eta t_{n} n^{b-1} \\
& \geq\|x-y\|\left(1-\frac{2 \sqrt{3} \eta n^{b-1}}{1-\frac{\lambda}{\sqrt{n}}}\right)
\end{aligned}
$$

Under the assumptions

$$
\begin{equation*}
n \geq 16|\log \varepsilon|^{2} \tag{26}
\end{equation*}
$$

and

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

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

$$
\operatorname{dist}\left(Q_{c}, Q_{s}\right) \geq\|x-y\|\left(1-\frac{\sqrt{3}}{2}|\log \varepsilon|^{-\frac{1}{2}}\right)
$$

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

$$
\begin{equation*}
\frac{1}{\operatorname{dist}\left(Q_{c}, Q_{s}\right)} \leq \frac{2}{\|x-y\|} \tag{27}
\end{equation*}
$$

Conditions (18) and (26) and the definition of $\lambda$ imply

$$
\frac{C_{2} \max \left\{L_{c}, L_{s}\right\} \lambda}{\Delta t n^{b}} \leq C_{3} \eta .
$$

Hence, from Theorem 12, we obtain the estimate

$$
\left|\check{\omega}_{n}^{\Delta t}(\|x-y\|)-\omega_{n}^{\Delta t}(\|x-y\|)\right| \leq \frac{C_{1}}{\operatorname{dist}\left(Q_{c}, Q_{s}\right)}\left(C_{3} \eta\right)^{q+1} .
$$

Inserting (27) leads to

$$
\left|\check{\omega}_{n}^{\Delta t}(\|x-y\|)-\omega_{n}^{\Delta t}(\|x-y\|)\right| \leq \frac{2 C_{1}}{\|x-y\|}\left(C_{3} \eta\right)^{q+1}
$$

Finally, the condition $\eta_{0} \leq\left(2 C_{3}\right)^{-1}$ implies that the interpolation order

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

leads to an approximation which satisfies

$$
\left|\check{\omega}_{n}^{\Delta t}(\|x-y\|)-\omega_{n}^{\Delta t}(\|x-y\|)\right| \leq \frac{2 C_{1} \varepsilon}{\|x-y\|}
$$

In [16] 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 (25), we directly obtain a similar convergence theorem also for the panel clustering method. In the following, we denote by $\tilde{\phi}_{\Delta t, k}^{n}$ the solution at time $t_{n}$ of the Galerkin discretization with cutoff strategy and panel clustering.
Theorem 15. Let the assumption of Theorem 14 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 $C>0$, such that for all cutoff parameters $\varepsilon$ in (9) such that $0<\varepsilon<C h \Delta t^{3}$ and interpolation orders $q \geq|\log \varepsilon| / \log 2$, the solution $\tilde{\phi}_{\Delta t, h}^{n}$ with cutoff and panel clustering satisfies the error estimate

$$
\left\|\tilde{\phi}_{\Delta t, h}^{n}-\phi\left(\cdot, t_{n}\right)\right\|_{H^{-1 / 2}(\Gamma)} \leq C_{g}(T)\left(\varepsilon h^{-1} \Delta t^{-5}+\Delta t^{2}+h^{m+3 / 2}\right) .
$$

Corollary 16. Let the assumptions of Theorem 15 be satisfied. Let $\Delta t \sim h^{m+3 / 2}$ and choose $\varepsilon \sim h^{7 m / 2+25 / 4}$. Then, the solution $\tilde{\phi}_{\Delta t, h}$ exists and converges with optimal rate

$$
\left\|\tilde{\phi}_{\Delta t, h}^{n}-\phi\left(\cdot, t_{n}\right)\right\|_{H^{-1 / 2}(\Gamma)} \leq C_{g}(T) h^{m+3 / 2} \sim C_{g}(T) \Delta t^{2}
$$

### 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 (18) (cf. Remark 10).

## Sparse approximation of the system matrix $\tilde{\mathbf{A}}_{n}$

To simplify the complexity analysis we assume that only the simple cutoff strategy and not the panel clustering method is applied for the first time steps:

$$
\begin{equation*}
0 \leq n \leq n^{p c} \tag{28}
\end{equation*}
$$

By using (13) and (14), the number of nonzero entries of all $\tilde{\mathbf{A}}_{n}$ in the case (28) is estimated from above by $\mathcal{O}\left(N M^{\frac{7}{8}} \log ^{6} M\right)$ and $\mathcal{O}\left(N M^{1+\frac{3}{8}} \log ^{11} M\right)$ ) for $m=0$ and $m=1$, respectively.

## 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. (22)) are computed recursively by using the tree structure. The details can be found in [17], [27]. In [17], it is shown that the computational and storage complexity is negligible compared to the generation of the influence matrices $\mathbf{S}_{(c, s)}$ (cf. (22)).

## Computation of the Influence Matrices

First, we compute the cardinality of $\mathcal{P}_{\varepsilon, n}^{\mathrm{pc}}$. Note that the maximal diameter of a cluster $c$ satisfying condition (18) is bounded by

$$
\begin{equation*}
L_{c} \leq \eta \frac{\Delta t n^{b}}{|\log \varepsilon|} \tag{29}
\end{equation*}
$$

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

$$
\left|\left\{(x, y) \in \Gamma \times \Gamma \mid\|x-y\| \in I_{n, \varepsilon}^{\Delta t}\right\}\right|=\mathcal{O}\left(\sqrt{\Delta t} t_{n}^{3 / 2}|\log \varepsilon|\right)
$$

where $|\omega|$ denotes the area measure of some $\omega \subset \Gamma \times \Gamma$ (cf. [17]) and that not only inequality (29) but also the reverse inequality holds for some other constant $\eta^{\prime}$. Hence, for sufficiently small $\Delta t$ the number of pairs of clusters satisfying (18) is bounded by

$$
\begin{equation*}
\mathcal{O}\left(\frac{\sqrt{\Delta t} t_{n}^{3 / 2}|\log \varepsilon|}{\left(\eta^{\prime} \frac{\Delta t n^{b}}{|\log \varepsilon|}\right)^{4}}\right) \tag{30}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathcal{O}\left(\frac{n^{3 / 2-4 b}|\log \varepsilon|^{11}}{\eta^{\prime 4} \Delta t^{2}}\right) \tag{31}
\end{equation*}
$$

Using the relations as in Corollary 16

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

|  | full matrix representation | cutoff strategy | panel clustering+cutoff strategy |
| :---: | :---: | :---: | :---: |
| $m=0$ | $\mathcal{O}\left(N M^{2}\right)$ | $\mathcal{O}\left(N M^{1+\frac{13}{16}} \log M\right)$ | $\mathcal{O}\left(N M^{1-\frac{1}{16}}\|\log M\|^{11}\right)$ |
| $m=1$ | $\mathcal{O}\left(N M^{2}\right)$ | $\mathcal{O}\left(N M^{1+\frac{11}{16}} \log M\right)$ | $\mathcal{O}\left(N M^{1+\frac{9}{16}}\|\log M\|^{11}\right)$ |

Table 2: Storage requirements for the panel clustering approximation and sparse approximation
we see that (31) is equivalent to (we use here $4 b=1$ )

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

To compute the total storage cost we sum over all $n \in\left\{n^{p c}, \ldots, N\right\}$ and obtain

$$
\begin{aligned}
\sum_{n=n^{p c}}^{N} n^{\frac{1}{2}}|\log \varepsilon|^{11} M^{\frac{m}{2}+\frac{3}{4}} & \leq C_{1} N^{\frac{3}{2}}|\log M|^{11} M^{\frac{m}{2}+\frac{3}{4}} \leq C_{2} N M^{\frac{5 m}{8}+\frac{15}{16}}|\log M|^{11} \\
& =C_{2}\left\{\begin{array}{cl}
N M^{\frac{15}{16}}|\log M|^{11} & m=0 \\
N M^{1+\frac{9}{16}}|\log M|^{11} & m=1
\end{array}\right.
\end{aligned}
$$

The total storage requirements are summarized in Table 5.3. The table shows that the panel clustering method combined with the cutoff strategy reduces the complexity of the space-time discretization of retarded integral equations significantly. For piecewise constant boundary elements we get a storage complexity with behaves even better than linearly, i.e., $\mathcal{O}(N M)$.

Remark 17. $\quad a$. The panel clustering method is based on a two-fold hierarchical structure ${ }^{1}$ : The clusters are organized in a cluster tree and the expansion system on each cluster are polynomials. Hence, by 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 $\left(n>n^{p c}\right)$, the integration of the highly oscillatory kernel functions is no longer necessary (cf. 23). Efficient quadrature methods for the integrals for $n<n^{p c}$ 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 the previous sections, 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 12.

[^1]In Remark 13, 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

$$
\begin{equation*}
|d-n| \leq \lambda \sqrt{n} \quad \text { with } \quad d=\|x-y\| / \Delta t \quad \text { and } \quad \lambda \text { as in (24). } \tag{32}
\end{equation*}
$$

Hence, we will investigate the function $\omega_{n}(d)$ only for values of $d$ which satisfy (32).
The estimates are obtained in several steps. In the first step, we consider the auxiliary functions

$$
\begin{equation*}
\tilde{\omega}_{n}(d):=4 \pi d \Delta t \omega_{n}^{\Delta t}(d \Delta t)=\frac{1}{n!}\left(\frac{d}{2}\right)^{\frac{n}{2}} e^{-\frac{3 d}{2}} H_{n}(\sqrt{2 d}) \tag{33}
\end{equation*}
$$

which are independent of $\Delta t$. We will determine bounds for the derivatives of $\tilde{\omega}_{n}(d)$ with respect to $d$ in Theorem 22 .

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 23.

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 [25]. The proof of the following lemma is postponed to the 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 18. The following estimates are valid for $x \geq 0$ and $n \geq 1$,

$$
\begin{equation*}
\left|e^{-\frac{x^{2}}{2}} H_{n}(x)\right| \leq C n!e^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{3}} \tag{34}
\end{equation*}
$$

and

$$
\begin{equation*}
\left|\partial_{x}\left(e^{-\frac{x^{2}}{2}} H_{n}(x)\right)\right| \leq C n!e^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{6}} \max \left\{\left|x^{2}-(2 n+1)\right|^{\frac{1}{4}} n^{-\frac{1}{12}}, x^{\frac{5}{12}} n^{-\frac{29}{24}}, 1\right\} \tag{35}
\end{equation*}
$$

With Lemma 18, we obtain the following estimate for $\tilde{\omega}_{n}(d)$ and $\tilde{\omega}_{n}^{\prime}(d)$.
Lemma 19. For $\tilde{\omega}_{n}(d)$ as defined in (33), the following bound holds for $n \geq 1$,

$$
\begin{equation*}
\left|\tilde{\omega}_{n}(d)\right| \leq C n^{-\frac{1}{3}}\left(\frac{d}{n}\right)^{\frac{n}{2}} e^{-\frac{d-n}{2}} \leq C n^{-\frac{1}{3}} \tag{36}
\end{equation*}
$$

For $n \geq 2$ and $|d-n| \leq \lambda \sqrt{n}$,

$$
\begin{equation*}
\left|\tilde{\omega}_{n}^{\prime}(d)\right| \leq C \lambda n^{-\frac{5}{8}}\left(\frac{d}{n}\right)^{\frac{n}{2}-1} e^{\frac{d-n}{2}} \leq C \lambda n^{-\frac{5}{8}} \tag{37}
\end{equation*}
$$

with $\lambda$ as in (24).

Proof. Due to (34), we have

$$
\left|\tilde{\omega}_{n}(d)\right|=\frac{1}{n!}\left(\frac{d}{2}\right)^{\frac{n}{2}} e^{-\frac{d}{2}}\left|e^{-d} H_{n}(\sqrt{2 d})\right| \leq C n^{-\frac{1}{3}}\left(\frac{d}{n}\right)^{\frac{n}{2}} e^{-\frac{d-n}{2}} .
$$

The last inequality in (36) follows from a straightforward analysis which shows that the maximum of $\left(\frac{d}{n}\right)^{\frac{n}{2}} e^{-\frac{d-n}{2}}$ is taken at $n=d$ and hence

$$
\begin{equation*}
\left(\frac{d}{n}\right)^{\frac{n}{2}} e^{-\frac{d-n}{2}} \leq 1 \tag{38}
\end{equation*}
$$

For the first derivative, we have

$$
\begin{aligned}
& \tilde{\omega}_{n}^{\prime}(d)= \\
& \frac{1}{n!}\left(\left(\frac{d}{2}\right)^{\frac{n}{2}} e^{-\frac{d}{2}} \partial_{d}\left(e^{-d} H_{n}(\sqrt{2 d})\right)+\partial_{d}\left(\left(\frac{d}{2}\right)^{\frac{n}{2}} e^{-\frac{d}{2}}\right) e^{-d} H_{n}(\sqrt{2 d})\right) \\
& =\left.\frac{1}{n!}\left(\frac{d}{2}\right)^{\frac{n}{2}} e^{-\frac{d}{2}} \partial_{x}\left(e^{-\frac{x^{2}}{2}} H_{n}(x)\right)\right|_{x=\sqrt{2 d}}(2 d)^{-\frac{1}{2}}-\frac{1}{2}\left(\frac{d}{n}\right)^{-1}\left(\frac{d}{n}-1\right) \tilde{\omega}_{n}(d)
\end{aligned}
$$

With (35) and $|d-n| \leq \lambda \sqrt{n}$, we obtain

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

Finally, with (13)

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

and by using (38), we arrive at (37).

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

Lemma 20. For $n \in \mathbb{N}_{0}$, the following relation holds

$$
\begin{equation*}
\tilde{\omega}_{n}^{\prime}(d)=-\frac{3}{2} \tilde{\omega}_{n}(d)+2 \tilde{\omega}_{n-1}(d)-\frac{1}{2} \tilde{\omega}_{n-2}(d) \tag{39}
\end{equation*}
$$

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

Proof. We recall

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

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

$$
\begin{equation*}
e^{-\gamma(\zeta) d}=\sum_{n=0}^{\infty} \tilde{\omega}_{n}(d) \zeta^{n} . \tag{40}
\end{equation*}
$$

Differentiating both sides of (40) with respect to $d$, we obtain

$$
-\gamma(\zeta) e^{-\gamma(\zeta) d}=-\sum_{n=0}^{\infty} \tilde{\omega}_{n}(d) \gamma(\zeta) \zeta^{n}=\sum_{n=0}^{\infty} \tilde{\omega}_{n}^{\prime}(d) \zeta^{n}
$$

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 $H_{0}(x)=1, H_{1}(x)=2 x$ and for $n \geq 1$

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

Lemma 21. For $n \in \mathbb{N}_{\geq 1}$, the recursion

$$
\begin{equation*}
\tilde{\omega}_{n}(d)=\frac{d}{n}\left(2 \tilde{\omega}_{n-1}(d)-\tilde{\omega}_{n-2}(d)\right), \tag{41}
\end{equation*}
$$

holds.

Now we can prove a bound for the derivatives of $\tilde{\omega}_{n}(d)$.
Theorem 22. Let $\frac{n}{2} \geq q, n \geq 1$, and $|d-n| \leq \lambda \sqrt{n}$ with $\lambda$ as in (24). Then

$$
\begin{equation*}
\left|\tilde{\omega}_{n}^{(q)}(d)\right| \leq q!(C \lambda)^{q} n^{-a_{q}}\left(\frac{d}{n}\right)^{\frac{n}{2}-q} e^{-\frac{d-n}{2}} \leq q!(C \lambda)^{q} n^{-a_{q}} \tag{42}
\end{equation*}
$$

with

$$
a_{0}=\frac{1}{3}, a_{1}=\frac{5}{8}, \quad \text { and } \quad a_{q}= \begin{cases}a_{1}+\frac{q-1}{4}, & q \text { odd },  \tag{43}\\ a_{0}+\frac{q}{4}, & q \text { even },\end{cases}
$$

and a generic constant $c$.

Proof. The proof is done by induction. For $q=0$ and $q=1$, the statement follows from Lemma 19.

Next, we show the statement for $q=2$. For simplicity, we omit the argument $d$ in $\tilde{\omega}_{n}(d)$ and $\tilde{\omega}_{n}^{\prime}(d)$. When differentiating (39), we obtain (recall $\tilde{\omega}_{-1}=\tilde{\omega}_{-2}=0$ )

$$
\begin{equation*}
\tilde{\omega}_{n}^{\prime \prime}=-\frac{3}{2}\left(\tilde{\omega}_{n}^{\prime}-\tilde{\omega}_{n-1}^{\prime}\right)+\frac{1}{2}\left(\tilde{\omega}_{n-1}^{\prime}-\tilde{\omega}_{n-2}^{\prime}\right) . \tag{44}
\end{equation*}
$$

Using (39) and (41), we obtain (recall $n \geq 1$ )

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

Thus

$$
\begin{align*}
\tilde{\omega}_{n}^{\prime}-\tilde{\omega}_{n-1}^{\prime} & =\left(\frac{d}{n}-1\right)\left(\tilde{\omega}_{n-1}^{\prime}-\frac{3}{2} \tilde{\omega}_{n-1}+\frac{1}{2} \tilde{\omega}_{n-2}\right)+\frac{1}{2 n} \tilde{\omega}_{n-1} \\
& =\left(\frac{d}{n}-1\right)\left(-3 \tilde{\omega}_{n-1}+\frac{5}{2} \tilde{\omega}_{n-2}-\frac{1}{2} \tilde{\omega}_{n-3}\right)+\frac{1}{2 n} \tilde{\omega}_{n-1} \tag{45}
\end{align*}
$$

By using $\left|\frac{d}{n}-1\right| \leq \lambda n^{-\frac{1}{2}}$ and Lemma 19, we obtain

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

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

$$
\begin{equation*}
\max _{k=1,2,3} \sup _{n \geq k+1}\left(\frac{n-k}{n}\right)^{-\alpha}=2^{\alpha} \quad \text { and } \max _{k=1,2,3} \sup _{n \geq k+1}\left(\frac{n}{n-k}\right)^{\frac{n-k}{2}}=e^{3 / 2} \tag{46}
\end{equation*}
$$

and, hence,

$$
\left|\tilde{\omega}_{n}^{\prime}-\tilde{\omega}_{n-1}^{\prime}\right| \leq C \lambda n^{-\frac{1}{2}-\frac{1}{3}} e^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n-3}{2}}
$$

Using (44), (46), and Lemma 19, we obtain

$$
\begin{equation*}
\left|\tilde{\omega}_{n}^{\prime \prime}\right| \leq C \lambda n^{-a_{2}} e^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n}{2}-2} \tag{47}
\end{equation*}
$$

with

$$
a_{2}=a_{0}+\frac{1}{2} .
$$

For the induction step $q \rightarrow q+1$, we assume that (42) holds for $q$. To show that (42) also holds for $q+1$, we first differentiate (39) $q$ times to obtain

$$
\begin{equation*}
\tilde{\omega}_{n}^{(q+1)}=-\frac{3}{2}\left(\tilde{\omega}_{n}^{(q)}-\tilde{\omega}_{n-1}^{(q)}\right)+\frac{1}{2}\left(\tilde{\omega}_{n-1}^{(q)}-\tilde{\omega}_{n-2}^{(q)}\right) . \tag{48}
\end{equation*}
$$

Furthermore, by differentiating (45), we get

$$
\begin{align*}
\tilde{\omega}_{n}^{(q)}-\tilde{\omega}_{n-1}^{(q)} & =\frac{q-1}{n}\left(-3 \tilde{\omega}_{n-1}^{(q-2)}+\frac{5}{2} \tilde{\omega}_{n-2}^{(q-2)}-\frac{1}{2} \tilde{\omega}_{n-3}^{(q-2)}\right)+\frac{1}{2 n} \tilde{\omega}_{n-1}^{(q-1)} \\
& +\left(\frac{d}{n}-1\right)\left(-3 \tilde{\omega}_{n-1}^{(q-1)}+\frac{5}{2} \tilde{\omega}_{n-2}^{(q-1)}-\frac{1}{2} \tilde{\omega}_{n-3}^{(q-1)}\right) . \tag{49}
\end{align*}
$$

Taking into account (32) and the induction assumption we get

$$
\begin{aligned}
\left|\tilde{\omega}_{n}^{(q)}-\tilde{\omega}_{n-1}^{(q)}\right| & \leq c_{1}\left\{\frac{q-1}{n}\left(\left|\tilde{\omega}_{n-1}^{(q-2)}\right|+\left|\tilde{\omega}_{n-2}^{(q-2)}\right|+\left|\tilde{\omega}_{n-3}^{(q-2)}\right|\right)\right. \\
& \left.+\lambda n^{-\frac{1}{2}}\left(\left|\tilde{\omega}_{n-1}^{(q-1)}\right|+\left|\tilde{\omega}_{n-2}^{(q-1)}\right|+\left|\tilde{\omega}_{n-3}^{(q-1)}\right|\right)\right\} \\
& \leq c_{1}\left\{\frac{(q-1)!}{n}(C \lambda)^{q-2} e^{-\frac{d-n}{2}} \sum_{k=1}^{\min \{n-1,3\}}(n-k)^{-a_{q-2}}\left(\frac{d}{n-k}\right)^{\frac{n-k}{2}-q+2}\right. \\
& \left.+\lambda n^{-\frac{1}{2}}(q-1)!(C \lambda)^{q-1} e^{-\frac{d-n}{2}} \sum_{k=1}^{\min \{n-1,3\}}(n-k)^{-a_{q-1}}\left(\frac{d}{n-k}\right)^{\frac{n-k}{2}-q+1}\right\} \\
& \stackrel{(46)}{\leq} c_{1}(q+1)!(C \lambda)^{q} e^{-\frac{d-n}{2}}\left(\frac{d}{n}\right)^{\frac{n-3}{2}-q+1}\left\{n^{-a_{q-2}-1}+n^{-a_{q-1}-\frac{1}{2}}\right\} .
\end{aligned}
$$

The combination with (48) yields

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

with

$$
a_{q}=\min \left\{a_{q-2}+\frac{1}{2}, a_{q-3}+1\right\}= \begin{cases}a_{1}+\frac{q-1}{4}, & q \text { odd } \\ a_{0}+\frac{q}{4}, & q \text { even }\end{cases}
$$

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

Table 3: $\tilde{a}_{q}$ for $0 \leq q \leq 6$

We have computed the maximum of the derivatives in numerical experiments to verify the sharpness of estimate (42). 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 $\tilde{a}_{q}=-\log \left(\frac{\left\|\tilde{\omega}_{40}^{(q)}(d)\right\|_{\infty}}{\left\|\tilde{\omega}_{600}^{(q)}(d)\right\|_{\infty}}\right) / \log (2 / 3)$. It can be seen that $\tilde{a}_{q} \approx 0.33+0.3 q$, i.e., $b \approx 0.3$ which compares well with the theoretical result $b \geq 0.25$.

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 23. For $\frac{n}{2} \geq q$ and $\left|\frac{\|x-y\|}{\Delta t}-n\right| \leq \lambda \sqrt{n}$ with $\lambda$ as in (24), we have

$$
\begin{aligned}
\left|\partial_{x_{i}}^{q} \omega_{n}^{\Delta t}(\|x-y\|)\right| & \leq \frac{(C \lambda)^{q} q!}{4 \pi\|x-y\|} \Delta t^{-q} n^{-a_{q}}\left(\frac{\|x-y\|}{n \Delta t}\right)^{\frac{n}{2}-q} e^{-\frac{\|x-y\|}{\Delta t}-n} \\
& \leq \frac{(C \lambda)^{q} q!}{\|x-y\|} \Delta t^{-q} n^{-a_{q}}
\end{aligned}
$$

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

For the proof of Theorem 23, we need the following lemma.
Lemma 24. Let $d=d(x, y)=\sqrt{\sum_{i=1}^{3}\left(x_{i}-y_{i}\right)^{2}}$. For a function $f(d)$, we have for $q \geq 1$,

$$
\left|\partial_{x_{i}}^{q} f(d)\right| \leq C^{q} q!\max _{1 \leq \nu \leq q} \frac{1}{\nu!}\left|f^{(\nu)}(d)\right| \frac{1}{d^{q-\nu}}
$$

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 $q \geq 2$ and $1 \leq \nu \leq q$,

$$
g_{\nu, q}(x, y)=\partial_{x_{i}} g_{\nu, q-1}(x, y)+g_{\nu-1, q-1}(x, y) \frac{x_{i}-y_{i}}{d}
$$

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

$$
\begin{equation*}
g_{\nu, q}(x, y)=\sum_{\mu=0}^{\min \left\{\left\lfloor\frac{q}{2}\right\rfloor, q-\nu\right\}} \alpha_{\mu, \nu}^{q} \frac{\left(x_{i}-y_{i}\right)^{q-2 \mu}}{d^{2 q-\nu-2 \mu}}, \quad 1 \leq \nu \leq q \tag{50}
\end{equation*}
$$

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

Assume that (50) holds for some $q$. Then

$$
\begin{aligned}
& g_{\nu, q+1}(x, y)=\partial_{x_{i}} g_{\nu, q}(x, y)+g_{\nu-1, q}(x, y) \frac{x_{i}-y_{i}}{d} \\
& =\sum_{\mu=0}^{\min \left\{\left\lfloor\frac{q}{2}\right\rfloor, q-\nu\right\}}(q-2 \mu) \alpha_{\mu, \nu}^{q} \frac{\left(x_{i}-y_{i}\right)^{q-2 \mu-1}}{d^{2 q-\nu-2 \mu}} \\
& -\sum_{\mu=0}^{\left.\min \left\{\frac{q}{2}\right\rfloor, q-\nu\right\}}(2 q-\nu-2 \mu) \alpha_{\mu, \nu}^{q} \frac{\left(x_{i}-y_{i}\right)^{q+1-2 \mu}}{d^{2 q+2-\nu-2 \mu}} \\
& +\sum_{\mu=0}^{\min \left\{\left\lfloor\frac{q}{2}\right\rfloor, q-\nu\right\}} \alpha_{\mu, \nu-1}^{q} \frac{\left(x_{i}-y_{i}\right)^{q-2 \mu+1}}{d^{2 q-\nu+2-2 \mu}} \\
& =\sum_{\mu=0}^{\left.\min \left\{\frac{q+1}{2}\right\rfloor, q+1-\nu\right\}} \alpha_{\mu \nu}^{q+1} \frac{\left(x_{i}-y_{i}\right)^{(q+1)-2 \mu}}{d^{2(q+1)-\nu-2 \mu}}
\end{aligned}
$$

with

$$
\begin{equation*}
\alpha_{\mu, \nu}^{q+1}=(q-2(\mu-1)) \alpha_{\mu-1, \nu}^{q}-(2 q-\nu-2 \mu) \alpha_{\mu, \nu}^{q}+\alpha_{\mu, \nu-1}^{q}, \tag{51}
\end{equation*}
$$

where we set all coefficients $\alpha_{\mu, \nu}^{q}$ not occurring in (50) to 0 . Thus,
We show by induction that $\left|\alpha_{\mu, \nu}^{q}\right| \leq c_{1}^{q} \frac{(q-1)!}{\nu!}$ for some constant $c_{1}$. First, for $q=1$, we have $\alpha_{0,1}^{1}=1$.

Let $\left|\alpha_{\mu, \nu}^{q}\right| \leq c_{1}^{q(q-1)!} \frac{1}{\nu!}$ for some $q$. We use (51) and $\nu \leq q+1$ to obtain

$$
\left|\alpha_{\mu, \nu}^{q+1}\right| \leq 3 q c_{1}^{q} \frac{(q-1)!}{\nu!}+c_{1}^{q} \nu \frac{(q-1)!}{\nu!} \leq c_{1}^{q+1} \frac{q!}{\nu!}
$$

when choosing $c_{1}$ large enough. The combination with (50) results in

$$
\left|g_{\nu, q}(x, y)\right| \leq c_{1}^{q} \frac{q!}{\nu!} \frac{1}{d^{q-\nu}} .
$$

Using $q \leq 2^{q}$, we obtain

$$
\begin{aligned}
\left|\partial_{x_{i}}^{q} f(d)\right| & \leq q \max _{1 \leq \nu \leq q}\left|g_{\nu, q}(x, y)\right|\left|f^{(\nu)}(d)\right| \\
& \leq\left(2 c_{1}\right)^{q} q!\max _{1 \leq \nu \leq q} \frac{1}{\nu!}\left|f^{(\nu)}(d)\right| \frac{1}{d^{q-\nu}}
\end{aligned}
$$

## Proof of Theorem 23.

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

$$
\begin{equation*}
\partial_{d}^{q} \omega_{n}^{\Delta t}(d)=\frac{1}{4 \pi d} \frac{1}{\Delta t^{q}} \sum_{l=0}^{q} \frac{q!}{l!}\left(-\frac{d}{\Delta t}\right)^{l-q} \tilde{\omega}_{n}^{(l)}\left(\frac{d}{\Delta t}\right) \tag{52}
\end{equation*}
$$

For $q=0$, the statement of the theorem follows easily by combining (36) with (52). For $q \geq 1$, from Theorem 22 and Lemma 24, we conclude that (recall $n / 2 \geq q$ )

$$
\begin{aligned}
& \left|\partial_{x_{i}}^{q} \omega_{n}^{\Delta t}(d)\right| \leq C^{q} q!\max _{1 \leq \nu \leq q} \frac{1}{\nu!}\left|\partial_{d}^{\nu} \omega_{n}^{\Delta t}(d)\right| d^{-q+\nu} \\
& \leq \frac{C^{q} q!}{4 \pi d} \max _{1 \leq \nu \leq q} \frac{1}{\Delta t^{\nu}} \sum_{l=0}^{\nu} \frac{1}{l!}\left(\frac{d}{\Delta t}\right)^{l-\nu} d^{-q+\nu}\left|\tilde{\omega}_{n}^{(l)}\left(\frac{d}{\Delta t}\right)\right| \\
& \leq \frac{C^{q} q!}{4 \pi d} \max _{1 \leq \nu \leq q} \sum_{l=0}^{\nu}(C \lambda)^{l} d^{l-q} n^{-a_{l}} \Delta t^{-l}\left(\frac{d}{n \Delta t}\right)^{\frac{n}{2}-l} e^{-\frac{d}{\Delta t}-n} 2 \\
& =\frac{C^{q} q!}{4 \pi d} \Delta t^{-q}\left(\frac{d}{n \Delta t}\right)^{\frac{n}{2}-q} e^{-\frac{d}{\Delta t-n} 2} \max _{1 \leq \nu \leq q} \sum_{l=0}^{\nu}(C \lambda)^{l} n^{-a_{l}-q+l} .
\end{aligned}
$$

From (43), it is easy to see

$$
a_{q}-a_{l}-q+l \leq 0
$$

and, hence,

$$
\left|\partial_{x_{i}}^{q} \omega_{n}^{\Delta t}(d)\right| \leq \frac{C^{q} q!}{4 \pi d} \Delta t^{-q}\left(\frac{d}{n \Delta t}\right)^{\frac{n}{2}-q} e^{-\frac{\frac{d}{\Delta t}-n}{2}} n^{-a_{q}} \frac{(C \lambda)^{q+1}-1}{C \lambda-1}
$$

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

## 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 cutoff 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.

| M | $\mathbf{A}_{\text {full }}$ | $\mathbf{A}_{\text {sparse }}$ | rel. error |
| ---: | ---: | ---: | ---: |
| 8192 | 512 MB | 4.4 MB | $7.1 \mathrm{e}-3$ |
|  |  | 16.2 MB | $7.3 \mathrm{e}-4$ |
|  |  | 34 MB | $8.2 \mathrm{e}-5$ |
|  |  | 63.1 MB | $5.0 \mathrm{e}-6$ |
|  |  | 91.5 MB | $6.2 \mathrm{e}-7$ |
|  |  | 124 MB | $7.7 \mathrm{e}-8$ |

Table 4: Storage requirements for sparse approximation: $n=0, \Delta t=0.1$

| M | $\mathbf{A}_{\text {full }}$ | q | $\mathbf{A}_{p c}$ | rel. error |
| ---: | ---: | ---: | ---: | ---: |
| 32768 | 8192 MB | 3 | 22.6 MB | $2.0 \mathrm{e}-3$ |
|  |  | 4 | 139 MB | $8.0 \mathrm{e}-4$ |

Table 5: Storage requirements for panel clustering approximation : $n=15, \Delta t=0.2$

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 technnique 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 [13] 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 cutoff 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.

## A Proof of Lemma 18

Lemma 25. The following estimates are valid for $x \geq 0$ and $n \geq 1$,

$$
\left|e^{-\frac{x^{2}}{2}} H_{n}(x)\right| \leq C n!e^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{3}}
$$

| M | $\mathbf{A}_{\text {full }}$ | q | $\mathbf{A}_{p c}$ | rel. error |
| ---: | ---: | ---: | ---: | ---: |
| 32768 | 8192 MB | 3 | 22.6 MB | $5.0 \mathrm{e}-2$ |
|  |  | 4 | 139 MB | $1.7 \mathrm{e}-2$ |

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

$$
\left|\partial_{x}\left(e^{-\frac{x^{2}}{2}} H_{n}(x)\right)\right| \leq C n!e^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{6}} \max \left\{\left|x^{2}-(2 n+1)\right|^{\frac{1}{4}} n^{-\frac{1}{12}}, x^{\frac{5}{12}} n^{-\frac{29}{24}}, 1\right\}
$$

Proof. The proof employs some special functions. Recall the definition of the Airy function (cf. [30])

$$
\operatorname{Ai}(x):=\frac{1}{2 \pi i} \int_{-i \infty}^{i \infty} e^{x z-z^{3} / 3} d z \quad \forall x \in \mathbb{R}
$$

We introduce the function $\xi: \mathbb{R}_{\geq-1} \rightarrow \mathbb{R}$ by

$$
\xi(x):=\left\{\begin{aligned}
\left(\frac{3}{2}\right)^{\frac{2}{3}}\left(x\left(x^{2}-1\right)^{\frac{1}{2}}-\operatorname{arccosh}(x)\right)^{\frac{2}{3}}, & \text { for } x>1 \\
-\left(\frac{3}{2}\right)^{\frac{2}{3}}\left(\arccos (x)-x\left(1-x^{2}\right)^{\frac{1}{2}}\right)^{\frac{2}{3}}, & \text { for }-1 \leq x \leq 1
\end{aligned}\right.
$$

and the function $\Phi: \mathbb{R}_{>-1} \rightarrow \mathbb{R}$

$$
\Phi(x):=\left(\frac{\xi(x)}{x^{2}-1}\right)^{\frac{1}{4}}
$$

Note that the functions $\zeta$ in $[25,(8.0 .4,5)]$ and $\phi$ in [25, (8.0.6)] satisfy

$$
\zeta(x)=\left(n+\frac{1}{2}\right)^{\frac{2}{3}} \xi(y) \quad \text { and } \quad \phi(x)=2^{-\frac{1}{4}} \frac{\Phi(y)}{\left(n+\frac{1}{2}\right)^{\frac{1}{12}}}
$$

where here and in the sequel we employ the convention

$$
\begin{equation*}
y=\frac{x}{\sqrt{2 n+1}} . \tag{53}
\end{equation*}
$$

a. A straightforward but somewhat tedious analysis shows that $\xi \in C^{1}([-1, \infty[)$ and $\left.\left.\Phi \in C^{1}(]-1, \infty\right]\right)$. The function $\xi(x)$ tends to $+\infty$ as $x \rightarrow+\infty$ and $\Phi(x)$ is unbounded as $x \rightarrow-1$, see Figures $2(\mathrm{a})$ and $2(\mathrm{~b})$. Consequently, there exists a constant $C_{\Phi}$ such that

$$
\begin{equation*}
|\Phi(x)| \leq C_{\Phi} \quad \forall x \geq 0 \tag{54}
\end{equation*}
$$

Furthermore, there exists a constant $C_{\mathrm{Ai}}$ such that

$$
\begin{equation*}
|\operatorname{Ai}(x)| \leq C_{\mathrm{Ai}} \quad \forall x \in \mathbb{R} \tag{55}
\end{equation*}
$$

b. The function $\Phi: \mathbb{R}_{>-1} \rightarrow \mathbb{R}$ is strictly monotonously decreasing and is positive

$$
\begin{equation*}
\forall x>-1 \quad \Phi(x)>0 \tag{56}
\end{equation*}
$$


(a) The Airy function (solid line) and (b) The function $\Phi$ (solid line) and its its derivative (dashed line). derivative (dashed line).

Figure 2: The Airy function and the function $\Phi$

For large arguments, we have

$$
\Phi(x)=x^{-1 / 6}(C+g(x))
$$

with some $C>0$ and a continuous function $g(x)$ which vanishes at infinity. Hence,

$$
\begin{equation*}
\left|\Phi^{-1}(x)\right| \leq C x^{1 / 6} \quad \text { as } x \rightarrow+\infty \tag{57}
\end{equation*}
$$

The function $\xi: \mathbb{R}_{>-1} \rightarrow \mathbb{R}$ is strictly monotonously increasing and has a zero at $x=1$.
c. We use $[25,(8.12)]$ and employ, for the estimate of $\varepsilon_{1}$ therein, the combination of $[25$, (8.03)] and [25, (8.22)] with [25, (2.11)] and [25, pp. 750-751] to obtain

$$
\begin{equation*}
e^{-\frac{x^{2}}{2}} H_{n}(x)=(2 \pi)^{\frac{1}{2}} e^{-\frac{n}{2}-\frac{1}{4}}(2 n+1)^{\frac{n}{2}+\frac{1}{6}} \Phi(y)\left\{\Upsilon_{1}(y)+\mathcal{O}\left(n^{-1}\right)\right\} \tag{58}
\end{equation*}
$$

where $\Upsilon_{1}(y):=\operatorname{Ai}\left(\xi(y)\left(n+\frac{1}{2}\right)^{\frac{2}{3}}\right)$. Since $x \geq 0$ implies $y \geq 0$ we obtain from (54), (55), (58)

$$
\left|e^{-\frac{x^{2}}{2}} H_{n}(x)\right| \leq C e^{-\frac{n}{2}}(2 n)^{\frac{n}{2}} n^{\frac{1}{6}}
$$

and the first statement of the lemma is obtained using Stirling's formula

$$
\frac{e^{-n} n^{n}}{n!} \leq \frac{e^{-n} n^{n}}{\sqrt{2 \pi} n^{n+\frac{1}{2}} e^{-n}}=C n^{-\frac{1}{2}}
$$

d. Let $\Upsilon_{2}(y):=\operatorname{Ai}^{\prime}\left(\xi(y)\left(n+\frac{1}{2}\right)^{\frac{2}{3}}\right)$. The modulus $\left|\Upsilon_{2}\right|$ is bounded except for the case when the argument $z:=\xi(y)\left(n+\frac{1}{2}\right)^{\frac{2}{3}}$ tends to $-\infty$ (see [25, (2.0.4,5)]) which is equivalent to $-1<y<1$ and $n \rightarrow \infty$. In this case, the growth behaviour is given $\left|\Upsilon_{2}(y)\right| \leq C|z|^{1 / 4}($ see $[25,(2.0 .5)])$.
For $y \rightarrow \infty,\left|\Upsilon_{2}(y)\right|$ decays exponentially (see $[25,(2.0 .4)]$ ) since $z(y)$ as well as $\xi(y)$ tends to $+\infty$ if $y \rightarrow+\infty$ (cf. a.).
e. We take the derivative of $[25,(8.11)]$ and use $[25,(4.17)]$. As stated in [25], similar estimates as $[25,(8.22)]$ can be obtained for $\eta_{1}$ occuring in $[25,(4.17)]$. We obtain

$$
\begin{align*}
& \partial_{x}\left(e^{-\frac{x^{2}}{2}} H_{n}(x)\right)=(2 \pi)^{\frac{1}{2}} e^{-\frac{n}{2}-\frac{1}{4}}(2 n+1)^{\frac{n}{2}+\frac{1}{3}}(\Phi(y))^{-1} \\
& \times\left\{\Upsilon_{2}(y)+n^{-1} \eta_{n}(x)\right. \\
& \left.+\Phi^{\prime}(y) \Phi(y) 2^{-1}\left(n+\frac{1}{2}\right)^{-\frac{2}{3}}\left\{\Upsilon_{1}(y)+\mathcal{O}\left(n^{-1}\right)\right\}\right\} \tag{59}
\end{align*}
$$

where $\left|\eta_{n}(x)\right| \leq \max \left\{x^{\frac{1}{4}} n^{-\frac{1}{8}}, 1\right\}$. We have all ingredients to show the second statement. We apply Stirling's formula to (59) to obtain

$$
\begin{align*}
& \left|\partial_{x}\left(e^{-\frac{x^{2}}{2}} H_{n}(x)\right)\right| \leq C n!e^{\frac{n}{2}}\left(\frac{2}{n}\right)^{\frac{n}{2}} n^{-\frac{1}{6}}  \tag{60}\\
& \times\left(\left|\Phi(y)^{-1} \Upsilon_{2}(y)\right|+n^{-1}\left|\Phi(y)^{-1}\right| \max \left\{x^{\frac{1}{4}} n^{-\frac{1}{8}}, 1\right\}+n^{-\frac{2}{3}}\left|\Phi^{\prime}(y)\right|\right) .
\end{align*}
$$

From (56) we conclude that $\Phi(y)^{-1}$ exists for all $y$. To find a bound in terms of $n$, we consider the three terms in (60) separately. The term $\left|\Phi(y)^{-1}\right|$ is bounded for bounded $y$ and grows like $y^{\frac{1}{6}}$ (cf. (57)). We distinguish between two cases.
i. $x \geq 1$. In this case, $z=\xi(y)\left(n+\frac{1}{2}\right)^{\frac{2}{3}}$ is non-negative. Hence, the function $\Upsilon_{2}$ is bounded and decays exponentially as $y \rightarrow \infty$ (cf. Property (d)). As a consequence, the slow growth behaviour of $\Phi(y)^{-1}$ (cf. (57) is dominated by the decay of $\Upsilon_{2}$ and we have

$$
\left|\Phi(y)^{-1} \Upsilon_{2}(y)\right| \leq C
$$

ii. $0<x \leq 1$. In this case, the function $\Phi(y)^{-1}$ is uniformly bounded and we get by using Property (d)

$$
\left|\Phi(y)^{-1} \Upsilon_{2}(y)\right| \leq C\left|\xi(y)\left(n+\frac{1}{2}\right)^{\frac{2}{3}}\right|^{1 / 4} \leq C\left(n+\frac{1}{2}\right)^{\frac{1}{6}}|\xi(y)|^{1 / 4}
$$

A Taylor argument yields for, $0 \leq y \leq 1$,

$$
|\xi(y)| \leq C\left|y^{2}-1\right|
$$

Hence,

$$
\left|\Phi(y)^{-1} \Upsilon_{2}(y)\right| \leq C\left|y^{2}-1\right|^{\frac{1}{4}} n^{\frac{1}{6}} .
$$

From Property (a) we conclude that $\Phi^{\prime}(y)$ is uniformly bounded for all $y \geq 0$.
Summarizing, we have, for $y \geq 0$,

$$
\begin{aligned}
\left|\Phi(y)^{-1} \Upsilon_{2}(y)\right| & \leq C \max \left\{1,\left|y^{2}-1\right|^{\frac{1}{4}} n^{\frac{1}{6}}\right\} \\
\left|\Phi(y)^{-1}\right| & \leq C \max \left\{1, y^{\frac{1}{6}}\right\} \\
\left|\Phi^{\prime}(y)\right| & \leq C
\end{aligned}
$$

When inserting $y=\frac{x}{\sqrt{2 n+1}}$, we arrive at the second statement of the lemma.

## References

[1] A. Bamberger and T. Ha-Duong. Formulation variationelle espace-temps pour le calcul par potentiel retardé d'une onde acoustique. Math. Meth. Appl. Sci., 8:405-435 and 598-608, 1986.
[2] L. Banjai and S.A. Sauter. Rapid solution of the wave equation in unbounded domains. Technical Report 10, Institut fü Mathematik, Unversity Zürich, 2007. http://www.math.unizh.ch/fileadmin/math/preprints/10-07.pdf.
[3] B. Birgisson, E. Siebrits, and A.P. Pierce. Elastodynamic Direct Boundary Element Methods with Enhanced Numerical Stability Properties. Int. J. Numer. Meth. Eng., 46:871-888, 1999.
[4] M.J. Bluck and S.P. Walker. Analysis of Three-Dimensional Transient Acoustic Wave Propagation using the Boudary Integral Equation Method. Int. J. Numer. Meth. Eng., 39:1419-1431, 1996.
[5] M. Costabel. Developments in Boundary Element Methods for Time-Dependent Problems. In L. Jentsch and F. Tröltsch, editors, Problems and Methods in Mathematical Physics, pages 17-32, Leipzig, 1994. B.G. Teubner.
[6] P.J. Davies. Numerical stability and convergence of approximations of retarded potential integral equations. SIAM, J. Numer. Anal., 31:856-875, 1994.
[7] P.J. Davies. Averaging techniques for time marching schemes for retarded potential integral equations. Appl. Numer. Math., 23:291-310, 1997.
[8] P.J. Davies and D.B. Duncan. Stability and Convergence of Collocation Schemes for Retarded Potential Integral Equations. SIAM J. Numer. Anal., 42(3):1167-1188, 2004.
[9] Y. Ding, A. Forestier, and T. Ha-Duong. A Galerkin Scheme for the Time Domain Integral Equation of Acoustic Scattering from a Hard Surface. J. Acoust. Soc. Am., 86(4):1566-1572, 1989.
[10] A.A. Ergin, B. Shanker, and E. Michielssen. Fast analysis of transient acoustic wave scattering from rigid bodies using the multilevel plane wave time domain algorithm. J. Acoust. Soc. Am., 117(3):1168-1178, 2000.
[11] M.B. Friedman and R.P. Shaw. Diffraction of Pulses by Cylindrical Obstacles of Arbitrary Cross Section. J. Appl. Mech., 29:40-46, 1962.
[12] I. S. Gradshteyn and I.M. Ryzhik. Table of Integrals, Series, and Products. Academic Press, New York, London, 1965.
[13] L. Grasedyck. Adaptive recompression of $\mathcal{H}$-matrices for BEM. Computing, 74:205-223, 2005.
[14] T. Ha-Duong. On Retarded Potential Boundary Integral Equations and their Discretization. In M. Ainsworth, P. Davies, D. Duncan, P. Martin, and B. Rynne, editors, Computational Methods in Wave Propagation, volume 31, pages 301-336, Heidelberg, 2003. Springer.
[15] T. Ha-Duong, B. Ludwig, and I. Terrasse. A Galerkin BEM for transient acoustic scattering by an absorbing obstacle. Int. J. Numer. Meth. Engng, 57:1845-1882, 2003.
[16] W. Hackbusch, W. Kress, and S. Sauter. Sparse convolution quadrature for time domain boundary integral formulations of the wave equation. Technical Report 116, MPI for Mathematics in the Sciences, Leipzig, 2005. http://www.mis.mpg.de/preprints/2005/prepr2005_116.html.
[17] W. Hackbusch, W. Kress, and S. Sauter. Sparse convolution quadrature for time domain boundary integral formulations of the wave equation by cutoff and panel-clustering. In M. Schanz and O. Steinbach, editors, Boundary Element Analysis: Mathematical Aspects and Applications. Springer Lecture Notes in Applied and Computational Mechanics, 2006. To appear.
[18] W. Hackbusch and Z.P. Nowak. On the Fast Matrix Multiplication in the Boundary Element Method by Panel-Clustering. Numerische Mathematik, 54:463-491, 1989.
[19] E. Hairer, C. Lubich, and M. Schlichte. Fast numerical solution of nonlinear Volterra convolution equations. SIAM J. Sci. Stat. Comput., 6(3):532-541, 1985.
[20] T. Hohage and F.-J. Sayas. Numerical solution of a heat diffusion problem by boundary element methods using the Laplace transform. Numer. Math., 102(1):67-92, 2005.
[21] C. Lubich. Convolution quadrature and discretized operational calculus I. Numer. Math., 52:129-145, 1988.
[22] C. Lubich. Convolution quadrature and discretized operational calculus II. Numer. Math., 52:413-425, 1988.
[23] C. Lubich. On the multistep time discretization of linear initial-boundary value problems and their boundary integral equations. Numer. Math., 67:365-389, 1994.
[24] E.K. Miller. An overview of time-domain integral equations models in electromagnetics. J. of Electromagnetic Waves and Appl., 1:269-293, 1987.
[25] F.W.J. Olver. Error bounds for first approximations in turning-point problems. J. Soc. Indust. Appl. Math., 11(3):748-772, 1963.
[26] B.P. Rynne and P.D. Smith. Stability of Time Marching Algorithms for the Electric Field Integral Equation. J. of Electromagnetic Waves and Appl., 4:1181-1205, 1990.
[27] S. Sauter and C. Schwab. Randelementmethoden. Teubner, Leipzig, 2004.
[28] A. Schädle, M. López-Fernández, and C. Lubich. Fast and oblivious convolution quadrature. SIAM J. Sci. Comput., 28(2):421-438, 2006.
[29] D. Sheen, I.H. Sloan, and V. Thomée. A parallel method for time discretization of parabolic equations based on Laplace transformation and quadrature. IMA J. Numer. Anal., 23(2):269-299, 2003.
[30] O. Vallée and M. Soares. Airy Functions and Applications to Physics. Imperial College Press, 2004.


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[^1]:    ${ }^{1}$ In the context of $\mathcal{H}$-matrices this two-fold hierarchy is called $\mathcal{H}^{2}$ format.

