

Rapid solution of the wave equation in unbounded domains

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Abstract

In this paper we propose and analyze a new, fast method for the numerical solution of time domain boundary integral formulations of the wave equation. We employ Lubich's convolution quadrature method for the time discretization and a Galerkin boundary element method for the spatial discretization. The coefficient matrix of the arising system of linear equations is a triangular block Toeplitz matrix. Possible choices to solve the linear system arising from the above discretization include the use of FFT techniques and the use of data-sparse approximations. By using FFT techniques, the computational complexity can be reduced substantially while the storage cost stays unchanged and is, typically, high. Using data-sparse approximations the gain is reversed: the computational cost is (approximately) unchanged while the storage cost is reduced substantially.

The method proposed in this paper combines the advantages of these two approaches. First, the discrete convolution (related to the block Toeplitz system) is transformed to the (discrete) Fourier image, thereby arriving at a decoupled system of discretized Helmholtz equations with complex wavenumbers. A fast data-sparse (e.g. FMM, panel-clustering) method can then be applied to the transformed system. Additionally, significant savings can be achieved if the boundary data is smooth and time-limited. In this case the right-hand sides of many of the Helmholtz problems are almost zero and can hence be disregarded. Finally the proposed method is inherently parallel.

We analyze the stability and convergence of these methods, thereby deriving the choice of parameters that preserves the convergence rates of the unperturbed convolution quadrature. We also present numerical results which illustrate the predicted convergence behaviour.

1 Introduction

Boundary value problems governed by the wave equation

$$\partial_t^2 u - \Delta u = f$$

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arise in many physical applications such as electromagnetic wave propagation or the computation of transient acoustic waves. Since such problems are typically formulated in unbounded domains, the method of integral equations is an elegant tool to transform this partial differential equation to an integral equation on the bounded surface of the scatterer.

Although this approach goes back to the early 1960s (cf. [18]), the development of fast numerical methods for integral equations in the field of hyperbolic problems is still in its infancies compared to the multitude of fast methods for elliptic boundary integral equations (cf. [37] and references therein). Existing numerical discretisation methods include collocation methods with some stabilization techniques (cf. [6], [7], [13], [14], [15], [32], [36]) and Laplace-Fourier methods coupled with Galerkin boundary elements in space ([3], [11],[16], [19]). Numerical experiments can be found, e.g., in [20].

In [17] 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.

We here employ the convolution quadrature method for the time discretisation and a Galerkin boundary element method in space. The convolution quadrature method for the time discretisation has been developed in [28], [29], [30], [31]. It provides a straightforward way to obtain a stable time stepping scheme using the Laplace transform of the kernel function. For applications to problems such as viscoelastic and poroelastic continua see [39, 40, 41].

The coefficient matrix in the arising system of linear equation is a block-triangular Toeplitz matrix consisting of N blocks of dimension $M \times M$, where N denotes the number of time steps and M is the number of spatial degrees of freedom. Due to the non-localness of the arising boundary integral operators, the $M \times M$ matrix blocks are densely populated.

In the literature, there exist (at least) two alternatives to solve this system efficiently. In [23], FFT-techniques are employed which make use of the Toeplitz structure of the system matrix and the computational complexity is reduced to $\mathcal{O}((N \log^2 N) M^2)$, while the storage complexity stays at $\mathcal{O}(NM^2)$. In [22], [21], [27], the $M \times M$ block matrices are approximated by data sparse representations based on a cutoff and panel-clustering strategy. This leads to a significant reduction of the storage complexity while the computational complexity is reduced compared to the naive approach (cost: $\mathcal{O}(N^2M^2)$) but increased compared to the FFT approach.

Also the classical Galerkin discretization of the retarded boundary integral equation, see [3, 19], leads to a block Toeplitz system matrix where the matrix blocks are of size $M \times M$ and sparse. More precisely, the number of non-zero entries in the block Toeplitz matrix is, for piecewise constant boundary elements, of order $\mathcal{O}(M^2)$ and, for piecewise linear boundary elements, of order $\mathcal{O}(M^{2+\frac{1}{8}})$ for this approach. Here, the total cost for the computation of a full Galerkin approximation sums up to $\mathcal{O}(M^2N)$ for piecewise constant boundary elements and to $\mathcal{O}(N^2M^{3/2})$ for piecewise linear boundary elements. A drawback of this approach, however, is that the numerical quadrature for computing the coefficients of the system matrix has to be carried out on the intersections of the boundary element mesh with the discrete light cone. The stable handling of these intersections and the implementation is especially complicated for curved panels.

In this paper, we propose a new approach which combines the advantages of the FFT-technique with the sparse approximation. We transfer the block Toeplitz system to the Fourier image by the discrete Fourier transform and then face the problem of computing approximate solutions of Helmholtz problems at different (complex) wave numbers. These Helmholtz prob-

lems are fully decoupled and can hence be efficiently solved on parallel computers. Relatively standard, fast methods (e.g. fast multipole method, hierarchical matrices) for the solution of frequency domain scattering can effectively be applied to these problems; see [8, 34] and [4]. It may also be possible to further reduce the computational cost of assembling the matrices by using the techniques for multifrequency analysis described in [26, 43]. Further, we also show that if the boundary data is sufficiently smooth and compatible and of limited time duration, instead of N , only $\mathcal{O}(N^\epsilon)$, for any fixed $\epsilon > 0$, Helmholtz systems need to be solved. Our method is similar and shares some properties (the need to solve a series of elliptic problems and the intrinsic parallelizability) of certain methods for parabolic equations; see [25, 42]. A related, interesting variation of the convolution quadrature for convolution kernels whose Laplace transform is sectorial can be found in [38].

A short description of the results of this paper has been published in the proceedings of the Waves 2007 conference [5].

2 Integral Formulation of the Wave Equation

Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain with boundary Γ ; typically, e.g., in scattering problems, Ω is an unbounded domain. In this paper, we present efficient methods for numerically solving the homogeneous wave equation

$$\partial_t^2 u - \Delta u = 0 \quad \text{in } \Omega \times (0, T) \quad (2.1a)$$

with initial conditions

$$u(\cdot, 0) = \partial_t u(\cdot, 0) = 0 \quad \text{in } \Omega \quad (2.1b)$$

and boundary conditions

$$u = g \quad \text{on } \Gamma \times (0, T) \quad (2.1c)$$

on a time interval $(0, T)$ for some $T > 0$. For its solution, we employ an ansatz as a *single layer potential*

$$u(x, t) = \int_0^t \int_\Gamma k(x - y, t - \tau) \phi(y, \tau) d\Gamma_y d\tau, \quad (x, t) \in \Omega \times (0, T), \quad (2.2)$$

where $k(z, t)$ is the fundamental solution of the wave equation,

$$k(z, t) = \frac{\delta(t - \|z\|)}{4\pi\|z\|}, \quad (2.3)$$

$\delta(t)$ being the Dirac delta distribution. The ansatz (2.2) satisfies the homogeneous equation (2.1a) and the initial conditions (2.1b). The extension $x \rightarrow \Gamma$ is continuous and hence, the unknown density ϕ in (2.2) is determined via the boundary conditions (2.1c), $u(x, t) = g(x, t)$. This results in the boundary integral equation for ϕ ,

$$\int_0^t \int_\Gamma k(x - y, t - \tau) \phi(y, \tau) d\Gamma_y d\tau = g(x, t) \quad \forall (x, t) \in \Gamma \times (0, T). \quad (2.4)$$

Existence and uniqueness results for the solution of the continuous problem are proved in [30] and [3, Prop. 3].

3 Numerical Discretisation

3.1 Time Discretisation via Convolution Quadrature

For the time discretisation, we employ the convolution quadrature approach which has been developed by Lubich in [28], [29], [30], [31]. We do not recall the theoretical framework here, but directly apply the approach to the wave equation. We make use of the following notation for the time convolution:

$$V(\partial_t)\phi := \int_0^t v(t-\tau)\phi(\tau)d\tau,$$

where V denotes the Laplace transform of the operator v ; for reasons behind using this notation see [28]. Note that, for the retarded single layer potential (2.2) v is a parameter dependent integral operator, i.e., $(v(t-\tau)\phi(\tau))(x) = \int_{\Gamma} k(x-y, t-\tau)\phi(\tau, y)d\Gamma_y$ (where we write $\phi(\tau, y)$ for $(\phi(\tau))(y)$) and $V(s)$ is the Laplace transform of v given by (3.4).

To discretize the time convolution we split the time interval $[0, T]$ into $N + 1$ time steps of equal length $\Delta t = T/N$ and compute an approximate solution at the discrete time levels $t_n = n\Delta t$. The continuous convolution operator $V(\partial_t)$ at the discrete times t_n , is replaced by the discrete convolution operator, for $n = 0, 1, \dots, N$,

$$(V(\partial_t^{\Delta t})\phi^{\Delta t})(t_n) := \sum_{j=0}^n \omega_{n-j}^{\Delta t}(V)\phi^{\Delta t}(t_j). \quad (3.1)$$

The convolution weights $\omega_n^{\Delta t}(V)$ are defined below (see (3.3)); whenever the underlying operator, v respectively V , is clear from the context, we will write $\omega_n^{\Delta t}$. The time-discrete problem is given by: Find $\phi_j(\cdot) = \phi^{\Delta t}(\cdot, t_j)$, such that

$$\sum_{j=0}^n (\omega_{n-j}^{\Delta t}\phi_j)(x) = g_n(x), \quad n = 1, \dots, N, \quad x \in \Gamma, \quad (3.2)$$

where $g_n(x)$ is some approximation to $g(x, t_n)$, or $g(x, t_n)$ itself.

For the derivation and the general framework and various applications, we refer to [28], [29], [30], and for our concrete problem to [22]. If the time discretisation is related to the unconditionally stable BDF2 scheme, the convolution weights $\omega_n^{\Delta t}$ are implicitly defined by

$$V\left(\frac{\gamma(\zeta)}{\Delta t}\right) = \sum_{n=0}^{\infty} \omega_n^{\Delta t}\zeta^n, \quad |\zeta| < 1. \quad (3.3)$$

Here, $V(s) : H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma)$, $\text{Re } s > 0$, is the single layer potential for the Helmholtz operator $\Delta U - s^2U = 0$,

$$(V(s)\varphi)(x) = \int_{\Gamma} K(\|x-y\|, s)\varphi(y)d\Gamma_y, \quad \text{where } K(d, s) := \frac{e^{-sd}}{4\pi d}. \quad (3.4)$$

Note that, K is the Laplace transform of the original time-domain kernel function (2.3). The function $\gamma(\zeta)$ is the quotient of the generating polynomials of the BDF2 scheme and is given by

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

3.2 A decoupled system of Helmholtz problems

As recommended in [28, 30] the convolution weights $\omega_j^{\Delta t}$ can be numerically computed by applying the trapezoidal rule to its representation as a contour integral,

$$\omega_j^{\Delta t}(V) = \frac{1}{2\pi i} \oint_C \frac{V(\gamma(\zeta)/\Delta t)}{\zeta^{j+1}} d\zeta, \quad (3.5)$$

where C can be chosen as a circle centred at the origin of radius $\lambda < 1$. The approximate convolution weights are then given by the scaled inverse discrete Fourier transform

$$\omega_j^{\Delta t, \lambda}(V) := \frac{\lambda^{-j}}{N+1} \sum_{l=0}^N V(s_l) \zeta_{N+1}^{lj}, \quad \text{where } \zeta_{N+1} = e^{\frac{2\pi i}{N+1}}, \quad s_l = \gamma(\lambda \zeta_{N+1}^{-l})/\Delta t.$$

Let us extend the above two formulae to negative indices $j < 0$; note that this implies $\omega_j^{\Delta t} = 0$ for $j < 0$. As $N \rightarrow \infty$ or $\lambda \rightarrow 0$ we have $\omega_j^{\Delta t} - \omega_j^{\Delta t, \lambda} = \mathcal{O}(\lambda^{N+1})$, $j = -N, \dots, N$; see Proposition 5.4. By extending the sum in (3.1) to $j = N$ and substituting the approximate weights in (3.2) we obtain a new system of equations for the new unknown $\phi^{\Delta t, \lambda}$:

$$\left(V(\partial_t^{\Delta t, \lambda}) \phi^{\Delta t, \lambda} \right) (t_n) := \sum_{j=0}^N \omega_{n-j}^{\Delta t, \lambda}(V) \phi_j^\lambda = g_n, \quad n = 0, 1, \dots, N. \quad (3.6)$$

The effect of the approximation on the difference between $\phi^{\Delta t, \lambda}$ and $\phi^{\Delta t}$ is discussed later. Substituting the definition of $\omega^{\Delta t, \lambda}$ in (3.6) we obtain the system of equations

$$\frac{\lambda^{-n}}{N+1} \sum_{l=0}^N \left(V(s_l) \hat{\phi}_l \right) (x) \zeta_{N+1}^{nl} = g_n(x), \quad n = 0, 1, \dots, N, \quad (3.7)$$

where

$$\hat{\phi}_l := \sum_{j=0}^N \lambda^j \phi_j^\lambda \zeta_{N+1}^{-lj}.$$

Note that the inverse transform is given by

$$\phi_l^\lambda = \frac{\lambda^{-l}}{N+1} \sum_{j=0}^N \hat{\phi}_j \zeta_{N+1}^{lj}. \quad (3.8)$$

Now, notice that, after multiplying by λ^n , applying the discrete Fourier transform with respect to n to both sides gives $N+1$ decoupled problems:

$$\left(V(s_l) \hat{\phi}_l \right) (x) = \hat{g}_l(x), \quad \text{for all } x \in \Gamma, \quad (3.9)$$

where

$$\hat{g}_l(x) = \sum_{n=0}^N \lambda^n g_n(x) \zeta_{N+1}^{-ln}.$$

We have thereby reduced the problem of solving numerically the wave equation to a system of Helmholtz problems with complex wavenumbers s_l , $l = 0, 1, \dots, N$. An example of the range of frequencies is given in Figure 1.

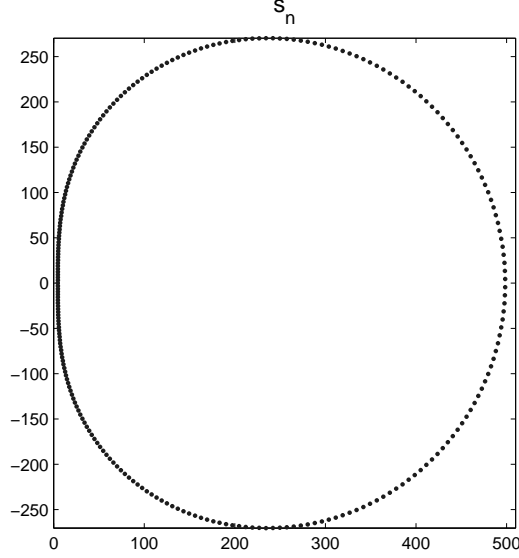


Figure 1: A range of complex frequencies for $N = 256$, $T = 2$, and $\lambda^N = 10^{-4}$. For this example it holds that $\text{Re } s_n > 4.6$, $n = 0, 1, \dots, N$.

Remark 3.1 *An important remark to make here is that*

$$V \left(\partial_t^{\Delta t, \lambda} \right) \phi^{\Delta t, \lambda} = g \quad \text{implies} \quad \phi^{\Delta t, \lambda} = V^{-1} \left(\partial_t^{\Delta t, \lambda} \right) g.$$

This can be seen by applying the scaled discrete inverse Fourier transform, see (3.8), to

$$\hat{\phi}_l = V^{-1}(s_l) \hat{g}_l,$$

thereby obtaining

$$\phi_n^\lambda = \frac{\lambda^{-n}}{N+1} \sum_{l=0}^N \hat{\phi}_l \zeta_{N+1}^{nl} = \frac{\lambda^{-n}}{N+1} \sum_{l=0}^N V^{-1}(s_l) \hat{g}_l \zeta_{N+1}^{nl} = \sum_{j=0}^N \omega_{n-j}^{\Delta t, \lambda} (V^{-1}) g_j.$$

The last step is obtained from the definition of \hat{g}_l and $\omega_n^{\Delta t, \lambda} (V^{-1})$; see also (3.6) and (3.7). This fact will help us in obtaining optimal error and stability estimates.

3.3 Spatial Discretization. Galerkin Boundary Element Methods

In the previous section we have derived the semi-discrete problem: For $n = 0, 1, \dots, N$, find $\phi_n^\lambda \in H^{-1/2}(\Gamma)$ such that

$$\sum_{j=0}^N \omega_{n-j}^{\Delta t, \lambda} \phi_j^\lambda = g_n, \quad n = 0, 1, \dots, N. \quad (3.10)$$

We have further shown that the above system is equivalent to a system of decoupled Helmholtz equations

$$\left(V(s_l) \hat{\phi}_l \right) (x) = \hat{g}_l(x), \quad \text{for all } x \in \Gamma. \quad (3.11)$$

In this paper we use a Galerkin boundary element method for the spatial discretization. Let \mathcal{G} be a regular (in the sense of Ciarlet [10]) boundary element mesh on Γ consisting of shape regular, possibly curved triangles. For a triangle $\tau \in \mathcal{G}$, the (regular) pull-back to the reference triangle $\hat{\tau} := \text{conv} \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$ is denoted by $\chi_\tau : \hat{\tau} \rightarrow \tau$. The space of piecewise constant, discontinuous functions is

$$S_{-1,0} := \{u \in L^\infty(\Gamma) \quad : \quad \forall \tau \in \mathcal{G} : u|_\tau \in \mathbb{P}_0\},$$

and, alternatively, we consider the space of continuous, piecewise linear functions

$$S_{0,1} := \{u \in C^0(\Gamma) \quad : \quad \forall \tau \in \mathcal{G} : (u \circ \chi_\tau)|_\tau \in \mathbb{P}_1\}$$

for the space discretisation. As a basis for $S_{-1,0}$, we choose the characteristic functions for the panels $\tau \in \mathcal{G}$, while the basis for $S_{0,1}$ consists of the standard hat functions, lifted to the surface Γ . The general notation is S for the boundary element space and $(b_m)_{m=1}^M$ for the basis. The mesh width is given by

$$h := \max_{\tau \in \mathcal{G}} h_\tau, \quad \text{where} \quad h_\tau := \text{diam}(\tau).$$

For the space-time discrete solution at time t_n we employ the ansatz

$$\phi_n^{h,\lambda}(y) = \sum_{m=1}^M \phi_{n,m} b_m(y), \quad (3.12)$$

where $(\phi_{n,m})_{m=1}^M \in \mathbb{R}^M$ are the nodal values of the discrete solution at time step t_n . Therefore, for the Helmholtz problems (3.11), the corresponding ansatz is

$$\hat{\phi}_l^h(y) = \sum_{m=1}^M \hat{\phi}_{l,m} b_m(y), \quad (3.13)$$

where the relationship between $\hat{\phi}_{l,m}$ and $\phi_{n,m}$ is given by $\hat{\phi}_{l,m} = \sum_{n=0}^N \lambda^n \phi_{n,m} \zeta_{N+1}^{ln}$.

To solve for the coefficients $\hat{\phi}_{l,m}$ we impose the integral equations (3.11) not pointwise but in a weak form: Find $\hat{\phi}_l^h \in S$ of the form (3.13) such that

$$\sum_{m=1}^M \hat{\phi}_{l,m} \int_\Gamma \int_\Gamma K(\|x - y\|, s_l) b_m(y) b_k(x) d\Gamma_y d\Gamma_x = \int_\Gamma \hat{g}_l(x) b_k(x) d\Gamma_x, \quad (3.14)$$

for $l = 0, 1, \dots, N$, $k = 1, 2, \dots, M$. Note that this is equivalent to imposing (3.10) in a weak form in order to compute $\phi_n^{h,\lambda}$.

4 Algorithmic Realization and Sparse Approximation

Applying the Galerkin boundary element method to the time-discrete equations (3.1) obtained by convolution quadrature, results in a block triangular, block Toeplitz system, each block being a dense Galerkin boundary element matrix; see [30] and [21]. This block system can be solved by using FFT techniques, see [23], with computational complexity of $\mathcal{O}(M^2 N \log^2 N)$ and a storage complexity of $\mathcal{O}(M^2 N)$. Alternatively (see [27]), one can approximate the

block matrices \mathbf{A}_n by a cutoff strategy and panel-clustering and directly solve the system without FFT. This reduces the storage cost significantly, while the computational complexity is $\mathcal{O}(M^2 N^{1+s})$, where the small value of s depends on the chosen discretisation. By rewriting (3.1) as a system of decoupled Helmholtz problems we are able to combine the advantages of both approaches.

We note that also the classical Galerkin discretization of the retarded boundary integral equation leads to a block Toeplitz system. Solving this system, see [3, 19], nevertheless results in suboptimal, higher than linear, computational complexity.

4.1 Reduction of the number of Helmholtz problems to be solved

A closer look at the Helmholtz problems tells us that only half of the problems need to be solved. Since $\hat{\phi}_l$, \hat{g}_l , and s_l are discrete Fourier transforms of real data, we know that they are, for $l = 1, 2, \dots, \lfloor \frac{N}{2} + 1 \rfloor$, the complex conjugates of $\hat{\phi}_j$, \hat{g}_j , s_j , for $j = \lceil \frac{N}{2} + 2 \rceil, \dots, N + 1$; for the case of s_l see Figure 1. Most importantly for us this means that

$$\hat{\phi}_{N+2-j} = \overline{\hat{\phi}_j}, \quad j = 1, 2, \dots, \left\lceil \frac{N}{2} + 1 \right\rceil. \quad (4.1)$$

Depending on the properties of the right-hand side g , it is possible to avoid the solution of a much larger number of Helmholtz problems without destroying the accuracy of the overall approximation. A particularly favourable case arises if g as a function of time can be extended to \mathbb{R} as a smooth function with support contained in $[0, T]$.

Let us assume that for some $x \in \Gamma$, $g(x, \cdot) \in C^\infty([0, T])$, and that

$$\partial_t^n g(x, 0) = \partial_t^n g(x, T) = 0, \quad \text{for all } n \in \mathbb{N}_0.$$

Further, define $g_\lambda(x, t) := \lambda^{t/\Delta t} g(x, t)$. Then it is clear that also $g_\lambda(x, \cdot) \in C^\infty([0, T])$ and that also all the partial derivatives with respect to time vanish at the end points of the time interval $[0, T]$. The reason for defining this function is that $\hat{g}_n(x)$ is an approximation of a Fourier coefficient of $g_\lambda(x, t)$ as we see next.

Let $g_\lambda(x, \cdot)$ be extended to the domain $[0, T + \Delta t]$ by zero (i.e. in a smooth way) and further extended to \mathbb{R} in a periodic way with period $T + \Delta t$. Let then

$$g_\lambda(x, t) = \sum_{j=-\infty}^{\infty} a_j e^{\frac{2\pi i j t}{T+\Delta t}}, \quad a_j = \frac{1}{T + \Delta t} \int_0^{T+\Delta t} g_\lambda(x, \tau) e^{\frac{-2\pi i j \tau}{T+\Delta t}} d\tau$$

be its Fourier expansion. Approximating the integral in the definition of the coefficients a_j by the trapezoidal rule we obtain exactly the values $\frac{1}{N+1} \hat{g}_j(x)$, where, assuming N even,

$$a_j \approx \frac{1}{N+1} \sum_{n=0}^N g_\lambda(x, t_n) e^{\frac{-2\pi i j n}{N+1}} = \frac{1}{N+1} \hat{g}_j(x), \quad \text{for } 0 \leq j \leq N/2.$$

See Figure 2 for an example of a right-hand side with the above properties and the decay of its Fourier coefficients. The solutions of Helmholtz problems with right-hand sides that are close to zero (all the right-hand sides on the central plateau in Figure 2) can be set to zero with no adverse affect on the accuracy of the overall method.

Remark 4.1 *A right-hand side g with the above properties can be thought of as a smooth signal of finite durability. If g does not have these properties it may still be possible to split the signal into a number of smooth and time limited signals.*

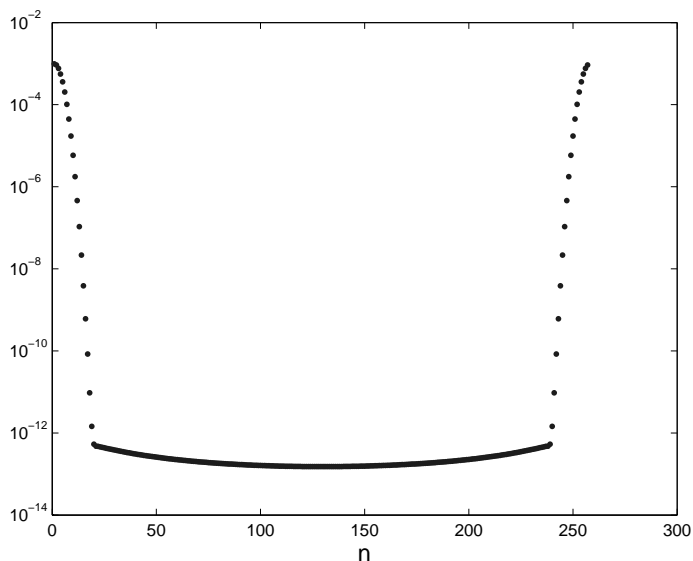


Figure 2: We plot $\max_{\|x\|=1} |\hat{g}_n(x)|$ for $N = 256$, $T = 2$, $\lambda^N = 10^{-8}$, and $g(t, x)$ the Gaussian pulse given by (6.5). The solution to the n th Helmholtz problem with n in the central plateau in the above plot, is accurately approximated by zero.

4.2 Data sparse approximation

To find a solution to (3.9) we need to solve a number of dense linear systems each of size $M \times M$. The cost of solving a single system by a direct method is $\mathcal{O}(M^3)$ and if a good preconditioner for an iterative method is available this can be reduced to $\mathcal{O}(M^2)$. In both cases the storage costs are $\mathcal{O}(M^2)$. The cost of recovering the values $\phi_{j,m}$ from $\hat{\phi}_{l,m}$ is negligible since it can be done exactly (if we ignore errors due to finite precision arithmetic) and efficiently using the FFT in time $\mathcal{O}(MN \log N)$; see also Remark 5.11.

One possibility for reducing these costs is to use panel-clustering or fast multipole techniques. We explain the basic idea behind these methods.

Let A_n be the n th linear system to be solved in (3.9), i.e.,

$$(A_n)_{kj} = \int_{\Gamma} \int_{\Gamma} K(\|x - y\|, s_n) b_j(y) b_k(x) d\Gamma_y d\Gamma_x.$$

Further we denote by \mathcal{I} the index set $\mathcal{I} := \{1, 2, \dots, M\}$ and refer to subsets $\tau \subset \mathcal{I}$ as *clusters* and define corresponding subsets of the boundary Γ by

$$\Gamma_{\tau} := \cup_{j \in \tau} \text{supp } b_j.$$

We call a pair of clusters $\tau \times \sigma$ a *block*. The corresponding block of the matrix A_n is then given by

$$(A_n|_{\tau \times \sigma})_{kj} = \begin{cases} (A_n)_{kj} & \text{if } k \in \tau \text{ and } j \in \sigma, \\ 0, & \text{otherwise.} \end{cases}$$

In the following definition, $B(c, r)$ denotes the ball centred at $c \in \mathbb{R}^3$ and radius $r > 0$.

Definition 4.2 A block $b = \tau \times \sigma$ is said to be η -admissible, for some $\eta < 1$, if there exist $r_\tau, r_\sigma > 0$ and $c_\tau, c_\sigma \in \mathbb{R}^3$ such that

$$r_\tau + r_\sigma \leq \eta \|c_\tau - c_\sigma\| \text{ and } \Gamma_\tau \subset B(c_\tau, r_\tau), \Gamma_\sigma \subset B(c_\sigma, r_\sigma).$$

For an admissible block our goal is to find a *separable* approximation of the fundamental solution:

$$K(|x - y|, s) \approx \sum_{l,k=1}^L u_k^\tau(x) s_{kl}^{\tau,\sigma} v_l^\sigma(y), \quad x \in \Gamma_\tau, y \in \Gamma_\sigma. \quad (4.2)$$

As indicated by the notation, we require that the basis functions $u_k^\tau(\cdot)$ (respectively $v_l^\sigma(\cdot)$) depend only on the cluster τ (respectively σ), and that the coefficients $s_{k,l}^b$ depend only on the block cluster $b = \tau \times \sigma$. Such an expansion allows us to approximate the block $A_n|_{\tau \times \sigma}$ of the matrix by a low rank matrix:

$$A_n|_{\tau \times \sigma} \approx USV^\top, \quad (4.3)$$

where

$$(U)_{kl} := \begin{cases} \int_{\Gamma_\tau} u_l^\tau(x) b_k(x) d\Gamma_x, & \text{if } k \in \tau, l = 1, \dots, L, \\ 0, & \text{otherwise,} \end{cases} \quad (4.4)$$

$$(V)_{jl} := \begin{cases} \int_{\Gamma_\sigma} v_l^\sigma(y) b_j(y) d\Gamma_y, & \text{if } j \in \sigma, l = 1, \dots, L, \\ 0, & \text{otherwise,} \end{cases} \quad (4.5)$$

and $(S)_{lm} := s_{lm}^{\tau,\sigma}$. Note that for $A_n|_{\tau \times \sigma}$ we need $O(|\tau||\sigma|)$ amount of storage, whereas for USV^\top $O(|\tau|L + |\sigma|L)$. If $L \ll \max\{|\tau|, |\sigma|\}$, it is significantly advantageous to use the low rank approximation of the block.

An extensive literature exists on the use of these methods to speed up the solution of the Helmholtz integral equations discretized by Galerkin boundary elements [2, 4, 12, 34, 35]. Most of this literature is however on the Helmholtz problem with a purely real wave number. For a purely real wave number the single layer potential representation is not always invertible, therefore certain stabilization methods need to be used. In our case the imaginary part of the wave number is strictly positive and we can use the single layer representation. The details of applying these “fast” methods to our case, together with algorithms and complexity estimates, will be given in a forthcoming paper. Here we investigate the effect of perturbations, due to the application of the fast methods, on the stability and accuracy. We assume that the kernel function $K(\cdot, s_l)$ in (3.9) is replaced by a separable approximation $K^{\text{pc}}(\cdot, s_l)$ such that

$$|K(d, s_l) - K^{\text{pc}}(d, s_l)| \leq \frac{\delta}{d}, \quad \text{for some } \delta > 0. \quad (4.6)$$

The solution of the resulting perturbed system is denoted by $\hat{\phi}_{l,m}^{\text{pc}}$. To obtain a uniform approximation (4.6) the length of expansion L needs to depend both on the block cluster $b = \tau \times \sigma$ and on s_l . Typically L is chosen so that

$$L \geq C \left(\text{Re } s_l \|c_\tau - c_\sigma\| + \log \frac{1}{\delta} \right)^{d-1}, \quad (4.7)$$

where C depends on the admissibility parameter η and $d = 2, 3$ is the space dimension. Explicit and sharp estimates on the optimal choice of L are difficult to obtain, especially for

complex wave numbers. In practice, one would estimate the error by a product of a Bessel and a Hankel function; see e.g. [1, 8]. Nevertheless, an important observation that can be made is that once L is greater than some threshold, the threshold depending on s_l , the convergence is exponential. This means that high accuracy can be obtained at little extra cost.

5 Error Analysis

In the previous section we have introduced a method to reduce the numerical solution of the wave equation to a system of Helmholtz problems. We have also described two ways of reducing the cost of solving these systems by introducing further approximations. In this section we investigate the stability and convergence of both the basic method and the further approximations. This allows us to adjust the control parameters of these methods to the required accuracy in an optimal way.

Let the approximation to the unknown density $\phi(x, t_n)$ obtained by the pure Lubich's method, i.e. with exact convolution weights, be given by $\phi_n^h \in S$. In [30] it is proved that if the data g is sufficiently smooth and compatible, then

$$\|\phi_n^h(\cdot) - \phi(\cdot, t_n)\|_{H^{-1/2}(\Gamma)} \leq C(\Delta t^2 + h^{m+3/2}), \quad (5.1)$$

where $m = 0$ for a piecewise constant basis and $m = 1$ for piecewise linear basis. By smooth and compatible we mean that $g \in H_0^5([0, T]; H^{1/2}(\Gamma))$ where

$$\begin{aligned} H_0^r([0, T]; H^{1/2}(\Gamma)) &:= \{g : \Gamma \times [0, T] \rightarrow \mathbb{R} : \text{there exists } g^* \in H^r(\mathbb{R}; H^{1/2}(\Gamma)) \\ &\quad \text{with } g = g^*|_{[0, T]} \text{ and } g^* \equiv 0 \text{ on } (-\infty, 0)\}, \\ H^r(\mathbb{R}; H^{1/2}(\Gamma)) &:= \left\{g : \Gamma \times \mathbb{R} \rightarrow \mathbb{R} : \int_{-\infty}^{\infty} (1 + |\omega|)^{2r} \|(\mathcal{F}g)(\cdot, \omega)\|_{H^{1/2}(\Gamma)}^2 d\omega < \infty\right\}, \end{aligned}$$

and \mathcal{F} denotes the integral Fourier transform with respect to the time variable $t \in \mathbb{R}$.

Our goal is to prove that the parameters in our method can be chosen so that convergence rates in (5.1) are preserved.

5.1 Errors due to the perturbation of $\omega_n^{\Delta t}$

Let $V_h(s) : S \rightarrow S$ be defined by

$$(V_h(s)\varphi, \psi)_{L^2(\Gamma)} := (V(s)\varphi, \psi)_{L^2(\Gamma)}, \quad \text{for all } \varphi, \psi \in S.$$

Whenever necessary, we will identify the inner product $(\cdot, \cdot)_{L^2(\Gamma)}$ with its extension to the dual pairing $H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)$. The solution by the convolution quadrature, i.e. with exact weights, is given by, see equation (5.5) in [30],

$$\phi^h = V_h^{-1}(\partial_t^{\Delta t})g^h$$

whereas with the perturbed weights the solution is given by

$$\phi_n^{h,\lambda} = \left(V_h^{-1}(\partial_t^{\Delta t, \lambda})g^h \right)(t_n),$$

(see Remark 3.1), where $g^h \in S$ is the L^2 -projection of g on S :

$$(g^h, \psi)_{L^2(\Gamma)} = (g, \psi)_{L^2(\Gamma)}, \quad \text{for all } \psi \in S.$$

For the remainder of the paper we will make use of the following notation:

$$\|\cdot\|_{+1} = \|\cdot\|_{H^{1/2}(\Gamma) \leftarrow H^{-1/2}(\Gamma)} \quad \text{and} \quad \|\cdot\|_{-1} = \|\cdot\|_{H^{-1/2}(\Gamma) \leftarrow H^{1/2}(\Gamma)}. \quad (5.2)$$

Lemma 5.1 *Let $\text{Re } s \geq \sigma_0 > 0$. Then*

$$\|V_h^{-1}(s)\|_{-1} \leq \frac{C_{stab}}{\min(1, \sigma_0)} |s|^2.$$

Proof. The result follows immediately from the definition of $V_h(s)$ and the coercivity estimate for $V(s)$ (see [3]):

$$\text{Re } (sV(s)\psi, \psi)_{L^2(\Gamma)} \geq C_{stab}^{-1} \frac{\min(1, \sigma_0)}{|s|} \|\psi\|_{H^{-1/2}(\Gamma)}^2.$$

■

Remark 5.2 *For $\omega \in \mathbb{R}$, there holds*

$$\begin{aligned} \gamma(\lambda e^{i\omega}) &= \frac{(\lambda + 3)(1 - \lambda) + 8(1 - \lambda)\lambda \sin^2 \frac{\omega}{2} + 8\lambda^2 \sin^4 \frac{\omega}{2}}{2} \\ &\quad - i\lambda \sin \omega \left(2(1 - \lambda) + \lambda \left(1 + 2 \sin^2 \frac{\omega}{2} \right) \right). \end{aligned}$$

For the real part, we obtain the estimate

$$\text{Re} \frac{\gamma(\lambda e^{i\omega})}{\Delta t} \geq \left(\frac{1 - \lambda}{2} + 4\lambda^2 \sin^4 \frac{\omega}{2} \right) / \Delta t.$$

For $0 \leq \lambda < 1$, we have the uniform bound with respect to ω .

$$\text{Re} \frac{\gamma(\lambda e^{i\omega})}{\Delta t} \geq \text{Re} \frac{\gamma(\lambda)}{\Delta t} = \frac{(3 + \lambda)(1 - \lambda)}{2\Delta t} \geq \frac{3(1 - \lambda)}{2\Delta t}.$$

For the modulus, the (rough) upper estimate holds

$$\left| \frac{\gamma(\lambda e^{i\omega})}{\Delta t} \right| \leq \frac{C}{\Delta t} \quad \text{with} \quad C = 5^{3/2}.$$

Lemma 5.3 *Let $W_h(s) := V_h^{-1}(s)/s^2$. Then,*

$$\|\omega_j^{\Delta t}(W_h)\|_{-1} \leq 2C_{stab}eT. \quad (5.3)$$

Further, for sufficiently smooth and compatible g , the identities

$$V_h^{-1}(\partial_t^{\Delta t})g = W_h(\partial_t^{\Delta t})((\partial_t^{\Delta t})^2g) \quad (5.4)$$

and, for $N \geq 4$,

$$V_h^{-1}(\partial_t^{\Delta t, \lambda})g = W_h(\partial_t^{\Delta t, \lambda})((\partial_t^{\Delta t})^2g), \quad (5.5)$$

hold, where $(\partial_t^{\Delta t})^2g$ denotes the two-fold application of the multistep approximation, in our case the BDF2 scheme.

Proof. The bound for $\|\omega_j^{\Delta t}(W_h)\|_{-1}$ follows from the Cauchy estimate by choosing the circle with radius $e^{-\Delta t/T}$ as the integration contour in (3.5), Remark 5.2, and Lemma 5.1:

$$\begin{aligned} \|\omega_j^{\Delta t}(W_h)\|_{-1} &\leq e^{j\Delta t/T} \max_{\|z\|=1} \|W_h(\gamma(e^{-\Delta t/T}z)/\Delta t)\|_{-1} \\ &\leq \frac{C_{\text{stab}}}{\min(1, (1 - e^{-\Delta t/T})/(2\Delta t))} e^{j\Delta t/T} \leq 2C_{\text{stab}}T e^{j/N}. \end{aligned}$$

Applying the (scaled) inverse discrete Fourier transform to the identity $V_h^{-1}(s_l)\hat{g}_l = W_h(s_l)s_l^2\hat{g}_l$, we see that $V_h^{-1}(\partial_t^{\Delta t, \lambda})g^h = W_h(\partial_t^{\Delta t, \lambda})\tilde{g}^h$ where

$$\tilde{g}_n^h = \frac{\lambda^{-n}}{N+1} \sum_{l=0}^{N+1} \hat{g}_l^h s_l^2 \zeta_{N+1}^{ln}, \quad s_l = \gamma(\lambda \zeta_{N+1}^{-l})/\Delta t.$$

The inverse discrete Fourier transform of s_l^2 is

$$\frac{1}{N+1} \sum_{l=0}^{N+1} (\gamma(\lambda \zeta_{N+1}^{-l})/\Delta t)^2 \zeta_{N+1}^{lj} \approx \frac{\lambda^j}{2\pi i} \oint_C \frac{(\gamma(\lambda \zeta)/\Delta t)^2}{\zeta^{j+1}} d\zeta = \frac{\lambda^j}{\Delta t^2} \delta_j \quad (5.6)$$

where

$$(\gamma(\zeta))^2 = \sum_{k=-\infty}^{\infty} \delta_k \zeta^k = \left(\frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2 \right)^2.$$

Since $(\gamma(\zeta))^2$ is a polynomial of order 4 and $N \geq 4$ the coefficients $\frac{\lambda^j}{\Delta t^2} \delta_j$ are reproduced exactly, without any quadrature error in (5.6). Therefore

$$\tilde{g}_n^h = \frac{1}{\Delta t^2} \sum_{j=0}^n \delta_{n-j} g_j^h$$

which is exactly the result of applying the BDF2 multistep method twice, where it is implicitly assumed that $g(t) = 0$ for $t \leq 0$. The result for $V_h^{-1}(\partial_t^{\Delta t})g^h$ is proved similarly, but with no restriction on N ; see also [30]. ■

Proposition 5.4 *Let $0 < \lambda < 1$. Then*

$$\|V_h^{-1}(\partial_t^{\Delta t})g^h - V_h^{-1}(\partial_t^{\Delta t, \lambda})g^h\|_{H^{-1/2}(\Gamma)} \leq 2C_{\text{stab}}eT^2 \frac{\lambda^{N+1}}{1 - \lambda^{N+1}} \Delta t^{-1}.$$

Proof. Let $a_j := \lambda^j \omega_j^{\Delta t}(W_h)$ and let $\hat{a}_j := \lambda^j \omega_j^{\Delta t, \lambda}(W_h)$, $W_h(s) = V_h^{-1}(s)/s^2$. Then \hat{a}_j is the discrete Fourier transform approximation to a_j for $j = -N, \dots, N$ and, see [24],

$$\begin{aligned} \|a_j - \hat{a}_j\|_{-1} &= \left\| \sum_{l=1}^{\infty} a_{j+l(N+1)} + a_{j-l(N+1)} \right\|_{-1} \leq \sum_{l=1}^{\infty} \|a_{j+l(N+1)}\|_{-1} \\ &\leq \lambda^j \sum_{l=1}^{\infty} \lambda^{l(N+1)} \|\omega_{j+l(N+1)}^{\Delta t}\|_{-1} \leq 2C_{\text{stab}}eT \lambda^j \frac{\lambda^{N+1}}{1 - \lambda^{N+1}}, \end{aligned}$$

where we have used the bound (5.3). Therefore

$$\|\omega_j^{\Delta t}(W_h) - \omega_j^{\Delta t, \lambda}(W_h)\|_{-1} \leq 2C_{\text{stab}}T \frac{\lambda^{N+1}}{1 - \lambda^{N+1}}$$

and the result follows from the definition of the discrete convolution and identities (5.4) and (5.5). ■

Theorem 5.5 *Let the exact solution $\phi(\cdot, t)$ be in $H^{m+1}(\Gamma)$ for any $t \in [0, T]$, data $g \in H_0^5([0, T]; H^{1/2}(\Gamma))$, $0 < \lambda < 1$, and let the boundary element space be $S = S_{m-1, m}$ for $m \in \{0, 1\}$. Then the discrete solution*

$$\phi_n^{h, \lambda} = \left(V_h^{-1}(\partial_t^{\Delta t, \lambda})g^h \right) (t_n)$$

satisfies the error estimate

$$\|\phi_n^{h, \lambda} - \phi(\cdot, t_n)\|_{H^{-1/2}(\Gamma)} \leq C_g \left(\frac{\lambda^{N+1}}{1 - \lambda^{N+1}} T^2 \Delta t^{-1} + \Delta t^2 + h^{m+3/2} \right),$$

where C_g depends on the right-hand side g , C_{stab} , and the time interval length T .

Proof. The result is a direct consequence of Proposition 5.4 and (5.1); see [30, Theorem 5.4].

■

5.2 Error due to the perturbation of $V_h(s)$

We investigate the effect of perturbing $V_h(s)$, in particular the effect of approximate evaluation of the kernel $K(d, s)$ by separable expansions. If these perturbations could be chosen analytic in s , then a stability and error estimate from Lemma 5.5 in [30] could be used in which there is no loss of powers of Δt . Unfortunately due to numerical stability issues, see [4, 8, 33], this is not the case for the problem at hand: different expansions need to be used for different values of s . Hence we will simply assume that

$$\|V_h^\varepsilon(s_l) - V_h(s_l)\|_{+1} \leq \varepsilon, \quad l = -N, -N+1, \dots, N-1, N \quad (5.7)$$

and investigate how this perturbation affects the final solution.

Lemma 5.6 *Let $\text{Re } s > \sigma_0 > 0$ and let $\varepsilon < \frac{1}{2} C_{stab}^{-1} \frac{\min(1, \sigma_0)}{|s|^2}$. Then $(V_h^\varepsilon(s))^{-1}$ is bounded and*

$$\|(V_h^\varepsilon(s))^{-1}\|_{-1} \leq 2C_{stab} \frac{|s|^2}{\min(1, \sigma_0)}.$$

Proof. Let us write

$$V_h^\varepsilon(s) = V_h(s) [I - V_h^{-1}(s)(V_h(s) - V_h^\varepsilon(s))].$$

From the estimate $\|V_h^{-1}(s)\|_{-1} \leq C_{stab}|s|^2/\min(1, \sigma_0)$, see Lemma 5.1, we see that $\varepsilon < \frac{1}{2} C_{stab}^{-1} \min(1, \sigma_0)/|s|^2$ is sufficient for $(V_h^\varepsilon(s))^{-1}$ to exist and to be bounded as above. ■

Lemma 5.7 *Let $\min_{l=0,1,\dots,N} \text{Re } s_l > \sigma_0 > 0$ and $\varepsilon < \frac{1}{2} C_{stab} \frac{\min(1, \sigma_0)}{\max_{l=0,1,\dots,N} |s_l|^2}$. Then*

$$\|\omega_j^{\Delta t, \lambda}(Q_h) - \omega_j^{\Delta t, \lambda}(Q_h^\varepsilon)\|_{-1} \leq CT \lambda^{-j} \varepsilon \Delta t^{-1},$$

where $C = \left(\frac{C_{stab}}{\min(1, \sigma_0)} \right)^2$,

$$Q_h(s) := \frac{V_h^{-1}(s)}{s^4}, \quad \text{and} \quad Q_h^\varepsilon(s) := \frac{(V_h^\varepsilon(s))^{-1}}{s^4}.$$

Proof. Using the fact $Q_h^{-1}(s) = s^4 V_h(s)$ we obtain the bound

$$\|Q_h(s_l) - Q_h^\varepsilon(s_l)\|_{-1} = \|Q_h(s_l)(s_l^4 V_h^\varepsilon(s_l) - s_l^4 V_h(s_l))Q_h^\varepsilon(s_l)\|_{-1} \leq \left(\frac{C_{stab}}{\min(1, \sigma_0)} \right)^2 \varepsilon.$$

From this and the definition of the perturbed convolution weights the result follows. ■

Let us define the solution of the ε -perturbed convolution equation by

$$\phi^{\lambda, h, \varepsilon} := (V_h^\varepsilon)^{-1}(\partial_t^{\Delta t, \lambda})g = Q_h^\varepsilon(\partial_t^{\Delta t, \lambda})((\partial_t^{\Delta t})^4 g)$$

and as before

$$\phi^{\lambda, h} := V_h^{-1}(\partial_t^{\Delta t, \lambda})g = Q_h(\partial_t^{\Delta t, \lambda})((\partial_t^{\Delta t})^4 g).$$

In the next result we estimate the difference between the two.

Proposition 5.8 *Let $\min_{l=0,1,\dots,N} \operatorname{Re} s_l > \sigma_0 > 0$ and $\varepsilon < \frac{1}{2} C_{stab} \frac{\min(1, \sigma_0)}{\max_{l=0,1,\dots,N} |s_l|^2}$ and let the data g be sufficiently smooth and compatible. Then*

$$\|\phi_n^{\lambda, h, \varepsilon} - \phi_n^{t, \lambda, h}\|_{H^{-1/2}(\Gamma)} \leq C \varepsilon T^2 \lambda^{-N} \Delta t^{-2},$$

with $C > 0$ as in Lemma 5.7.

Proof. The result is a direct consequence of the above lemma. ■

The above result together with Remark 5.2 implies that to obtain optimal convergence it is sufficient to insure that $\varepsilon \leq C \lambda^N \Delta t^4$.

Let us now investigate what is the effect of perturbations to the kernel function $K(d, s)$. In order to do this we assume

$$|K(\|x - y\|, s_l) - K^{pc}(\|x - y\|, s_l)| \leq \delta \frac{1}{\|x - y\|} \quad \text{for all } x, y \in \Gamma \quad (5.8)$$

for $l = 0, 1, \dots, N$, and define the operator $V_h^{pc}(s) : S \rightarrow S$ by

$$(V_h^{pc}(s)\psi, \varphi)_{L^2(\Gamma)} = \int_{\Gamma} \int_{\Gamma} K^{pc}(\|x - y\|, s) \psi(y) \overline{\varphi(x)} d\Gamma_y d\Gamma_x.$$

Proposition 5.9 *Let (5.8) hold. Then, there exists $C_0 > 0$ such that*

$$\|V_h^{pc}(s_l) - V_h(s_l)\|_{+1} \leq C_0 h^{-1} \delta.$$

Hence if $\delta \leq \frac{1}{2} C_0 C_{stab} h \frac{\min(1, \sigma_0)}{\max_l |s_l|^2} \leq Ch \Delta t^2$ we have the estimate

$$\|{}^{pc}\phi_n^{\lambda, h} - \phi_n^{\lambda, h}\|_{H^{-1/2}(\Gamma)} \leq C \delta T h^{-1} \lambda^{-N} \Delta t^{-2}$$

holds, where

$${}^{pc}\phi^{\lambda, h} = (V_h^{pc})^{-1}(\partial_t^{\Delta t, \lambda})g.$$

Proof. Let $\varphi \in S$. The well known L^2 -continuity of the single layer potential for the Laplacian and a scaling inequality for boundary element functions lead to

$$\begin{aligned} \|(V_h^{pc}(s_l) - V_h(s_l))\varphi\|_{H^{1/2}(\Gamma)} &\leq \delta \sup_{\substack{\psi \in S(\Gamma) \\ \|\psi\|_{H^{-1/2}(\Gamma)}=1}} \int_{\Gamma \times \Gamma} |\varphi(y)| |\psi(x)| \frac{1}{\|x - y\|} ds_x ds_y \\ &\leq C \delta \sup_{\substack{\psi \in S(\Gamma) \\ \|\psi\|_{H^{-1/2}(\Gamma)}=1}} \|\varphi\|_{L^2(\Gamma)} \|\psi\|_{L^2(\Gamma)} \leq Ch^{-1} \delta \|\varphi\|_{H^{-1/2}(\Gamma)}. \end{aligned}$$

The estimate of the error in the solution is then a direct consequence of Proposition 5.8 and Remark 5.2. ■

In the following result, the binary relation $A \lesssim B$ is used to denote the existence of a constant C independent of any discretization parameters such that $A \leq CB$. Further $A \sim B$ implies $A \lesssim B$ and $B \lesssim A$.

Corollary 5.10 *Let the conditions of Theorem 5.5 be satisfied, let (5.8) hold, and let*

$$h^{m+3/2} \lesssim \Delta t^2, \quad \lambda^{N+1} \sim \Delta t^3, \quad \delta \lesssim \lambda^N h \Delta t^4 \lesssim h^{7m/2+25/4}.$$

Then the optimal rate of convergence is achieved,

$$\|{}^{pc}\phi_n^{\lambda,h} - \phi(\cdot, t_n)\|_{H^{-1/2}(\Gamma)} \leq C \Delta t^2,$$

where C depends on the data g .

Remark 5.11 *According to the above result λ should be chosen as $\lambda \sim \Delta t^{3/(N+1)} = e^{\frac{3}{N+1} \log \frac{T}{N}}$. Since the rounding errors, in the same manner as the errors due to panel-clustering, are magnified by λ^{-j} , λ should be chosen in the interval $\sqrt{\text{eps}} < \lambda^N < 1$, where eps is the machine accuracy. In IEEE double precision this is approximately 10^{-16} , therefore the accuracy of the method is limited by the choice $\lambda > 10^{-8/N}$. This accuracy limit can however be improved if an n -trapezoidal rule is used to compute the weights $\omega_j^{\Delta t, \lambda}$ with $n = jN$, $j > 1$.*

Remark 5.12 *The condition on the accuracy of the panel-clustering approximation is rather stringent. However since the convergence of the separable expansion is exponential for large enough length of expansion L , see (4.7), the computational costs of the panel-clustering method depend only logarithmically on the required accuracy. Therefore the overall computational cost is not affected significantly.*

If we had assumed that $V_h^{pc}(s) - V_h(s)$ is analytic in s and could be bounded by $C|s|^2$, significantly better error estimates could be obtained by using Lemma 5.5 in [30]. Unfortunately, due to the well-known numerical stability issues with the multipole expansions for the Helmholtz kernel [4, 8, 33], different types of expansions need to be used in for different admissible block; the choice of the block depending on the wavenumber s_l . This restricts us from using the more favourable results of Lemma 5.5 in [30].

5.3 Error due to the reduction of the number of linear systems

Corollary 5.13 *Let $0 \leq \lambda < 1$ and $\sigma_l = \text{Re } s_l$. Then*

$$\|\hat{\phi}_l^h\|_{H^{-1/2}(\Gamma)} \leq C_1 (\Delta t)^{-2} \|\hat{g}_l\|_{H^{1/2}(\Gamma)},$$

where $C_1 = 5^3 \frac{C_{\text{stab}}}{\min(1, \sigma_l)}$.

Proof. The result is a direct consequence of Lemma 5.1 and Remark 5.2. ■

Let $\mathbf{N}_z \subset \{0, 1, \dots, N\}$ determine the Helmholtz problems the solution of which will be computed; the rest will be approximated by zero. Then we define the resulting approximation to $\phi^{h,\lambda}$ by

$$\emptyset \phi_n^{h,\lambda}(x) := \frac{\lambda^{-n}}{N+1} \sum_{l \in \mathbf{N}_z} \hat{\phi}_l^h(x) \zeta_{N+1}^{ln}.$$

Corollary 5.14 *Let $n \in \{0, 1, \dots, N\}$. If*

$$\max_{l \notin \mathbf{N}_z} \|\hat{g}_l\|_{H^{1/2}(\Gamma)} \leq C_1^{-1} \lambda^n (\Delta t)^4,$$

then we obtain optimal order convergence at time step t_n :

$$\|\hat{\phi}_n^{\emptyset, h, \lambda} - \phi_n^{h, \lambda}\|_{H^{-1/2}(\Gamma)} \leq \Delta t^2.$$

Proof. The proof follows directly from Corollary 5.13. ■

Next we show that if the right-hand side is smooth and of finite duration, it is sufficient to solve only a few Helmholtz systems. Let us introduce the space of functions that are zero at both $t = 0$ and $t = T$.

$$H_{00}^r([0, T]; H^{1/2}(\Gamma)) := \{g : \Gamma \times [0, T] \rightarrow \mathbb{R} : \text{there exists } g^* \in H^r(\mathbb{R}; H^{1/2}(\Gamma)) \\ \text{with } g = g^*|_{[0, T]} \text{ and } \text{supp } g^* \subset [0, T]\}.$$

Theorem 5.15 *Let $g \in H_{00}^r([0, T]; H^{1/2}(\Gamma))$ for some $r \geq 3.5$ and $\epsilon > 0$ be given. For any $N \in \mathbb{N}$ let $\lambda := \epsilon^{\frac{1}{N}}$. Then, \mathbf{N}_z can be chosen so that $\#\mathbf{N}_z \leq C \epsilon^{-\frac{1}{r+1/2}} N^{\frac{4}{r+1/2}}$ and the optimal order convergence is retained. The constant C depends on $r, (\log \epsilon)/T$, and g .*

Proof. Let $g_\lambda(x, t) := \lambda^{t/\Delta t} g(x, t) = \epsilon^{\frac{t}{T}} g(x, t) = e^{t \frac{\log \epsilon}{T}} g(x, t)$ on $t \in [0, T]$. Then we see that g_λ is independent of N and that $g_\lambda \in H_{00}^r([0, T]; H^{1/2}(\Gamma))$. Then for $\omega \in \mathbb{R}$, $\|(\mathcal{F}g_\lambda)(\cdot, \omega)\|_{H^{1/2}(\Gamma)} = o(|\omega|^{-r-1/2})$. Taking $\omega_j = 2\pi j/(T + \Delta t) = 2\pi j N/(T(N + 1))$ we define

$$a_j := \|(\mathcal{F}g_\lambda)(\cdot, \omega_j)\|_{H^{1/2}(\Gamma)} = o(j^{-r-1/2}), \quad j \in \mathbb{Z}.$$

Then using the aliasing formula, see [24], we arrive at an estimate for \hat{g}_n , for $n = 1, \dots, N/2 - 1$,

$$\|\hat{g}_n\|_{H^{1/2}(\Gamma)} \leq a_n + \sum_{k > N/2} a_k = o(n^{-r-1/2} + N^{-r+1/2}) = o(n^{-r-1/2}).$$

The constants in the $o(\cdot)$ notation depend only on $r, (\log \epsilon)/T$, ϵ , and g . The result now follows from Corollary 5.14. ■

6 Numerical experiments

In this section we present the results of numerical experiments. Except for one simple example, the experiments will be done in two dimensions. All the steps in the method remain the same in two dimensions except that the fundamental solution for the wave equation is given by

$$k_{2D}(d, t) = \frac{H(t-d)}{2\pi\sqrt{t^2-d^2}}, \quad (6.1)$$

where H is the Heaviside function:

$$H(t) = \begin{cases} 0, & \text{for } t < 0, \\ 1, & \text{for } t > 0. \end{cases}$$

The Laplace transform $K_{2D}(d, s)$ is again the fundamental solution of the Helmholtz equation $\Delta U - s^2 U$:

$$K_{2D}(d, s) = \frac{i}{4} H_0^{(1)}(isd), \quad (6.2)$$

where $H_0^{(1)}(\cdot)$ is the zero order Hankel function of first kind.

Let us consider the case of Γ being the unit ball in \mathbb{R}^2 or \mathbb{R}^3 and a right-hand side that is separable in the time and the spatial variables: $g(x, t) = g(t)e(x)$, where $e(x)$ is an eigenfunction of the single layer potential $V(s)$ with the eigenvalue $\lambda_l(s)$. In two dimensions the eigenfunctions are the complex exponentials $e^{il\theta}$ and $\lambda_l(s) = \frac{i\pi}{2} J_l(is)H_l(is)$ whereas in three dimensions these are the spherical harmonics $Y_l^m(\theta, \varphi)$ with $\lambda_l(s) = -sj_l(is)h_l(is)$; we have used the standard polar/spherical coordinates to describe the eigenfunctions. Here $J_l(\cdot)$, respectively $j_l(\cdot)$, are cylindrical, resp. spherical, Bessel functions of order l , whereas $H_l^{(1)}(\cdot)$, resp. $h_l^{(1)}(\cdot)$, are the cylindrical, resp. spherical, Hankel functions of first kind and order l . The problem of finding the unknown density $\phi(x, t)$ can then be reduced to the single, time, dimension. This can be seen by replacing the fundamental solution k in the single layer representation formula by the inverse Laplace transform of its Laplace transform K :

$$\begin{aligned} g(t)e(x) &= \int_0^t \int_{\Gamma} k(t - \tau, \|x - y\|) \phi(\tau, x) d\Gamma_y d\tau \\ &= \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \int_0^t e^{s\tau} \int_{\Gamma} K(s, \|x - y\|) \phi(t - \tau, y) d\Gamma_y d\tau ds \\ &= \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \int_0^t e^{s\tau} (V(s)\phi(t - \tau, \cdot))(x) d\tau ds, \quad x \in \Gamma, \text{ for some } \sigma > 0. \end{aligned}$$

Therefore, we can use the ansatz $\phi(x, t) = \phi(t)e(x)$ to reduced the problem to finding $\phi(t)$ such that

$$g(t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \int_0^t e^{s\tau} \lambda_l(is) \phi(t - \tau) d\tau ds.$$

Hence we need to solve a convolution integral equation in one dimension:

$$g(t) = \int_0^t \check{\lambda}_l(\tau) \phi(t - \tau) d\tau, \quad (6.3)$$

where $\check{\lambda}_l(\cdot)$ is the inverse Laplace transform of $\lambda_l(\cdot)$. The latter equation can then be solved by Lubich's original method, which makes use only of $\lambda_l(\cdot)$ and not its inverse Laplace transform. The first few numerical examples will be of this type.

6.1 Radial solution of scattering by unit sphere

In this example we consider the three dimensional case, $\Gamma = \mathbb{S}^2$. Let $g(x, t) = g(t)$ be constant for a fixed time t , i.e. $e(x) = 2\sqrt{\pi}Y_0^0 = 1$. In this particularly simple case it can be shown that

$$\phi(t) = 2g'(t), \quad t \in [0, 2].$$

The restriction to the interval $[0, 2]$ is a consequence of the fact that the diameter of the sphere is 2. For time $t > 2$ the expression for $\phi(t)$ is more complicated.

N	error	rate
4	1.44	-/-
8	0.45	1.68
16	0.12	1.90
32	0.032	1.94
64	0.0081	1.96
128	0.0020	1.99
256	0.00051	1.99
512	0.00013	2.00
1024	3.2×10^{-5}	2.00

Table 1: The results for scattering by unit sphere with $g(x, t) = \sin^5(t)$ and $\lambda = \Delta t^{3/N}$.

The right-hand side of the n th Helmholtz problem is a constant:

$$\hat{g}_n = \sum_{j=0}^N \lambda^j g(t_j) \zeta_{N+1}^{-nj},$$

and the solution of the Helmholtz problem is also a constant and is given by

$$\hat{\phi}_n = \frac{\hat{g}_n}{\lambda_0(s_n)}.$$

The approximation to the unknown density at time-step t_n is given by

$$\phi_n := \frac{\lambda^{-n}}{N+1} \sum_{j=0}^N \hat{\phi}_j \zeta_{N+1}^{nj}.$$

If λ is chosen small enough, theoretical estimates predict the following behaviour of the error:

$$\left(\sum_{n=0}^N \Delta t |\phi(t_n) - \phi_n|^2 \right)^{1/2} \leq C \Delta t^2.$$

One more detail needs to be fixed before the experiments can be started, namely the choice of λ . Recall that λ needs to be chosen small enough to insure stability and accuracy, see Theorem 5.5, but also large enough to avoid numerical instability issues, see Remark 5.11. As suggested in Remark 5.11 we make the choice

$$\lambda = \max(\Delta t^{3/N}, \text{eps}^{\frac{1}{2N}}). \quad (6.4)$$

Numerical results for the scattering by unit sphere are given in Table 1 and show that our theoretical estimates are sharp for this example.

6.2 A non-radial example

In this example we consider the two dimensional case. We pick the right-hand side to be $g(x, t) = h(t) \cos(l\theta)$, where for the space variable we use the polar coordinate system $r \in \mathbb{R}_{\geq 0}$,

N	M	$\ \phi - \phi^{h,\lambda}\ _{-1/2,l^2}$	rate
4	16	0.78	-/-
8	40	0.27	1.54
16	102	0.084	1.68
32	254	0.023	1.83
64	640	0.0062	1.93
128	1610	0.0016	1.98

Table 2: The results for scattering by the unit disk with $g(x, t) = \sin^5(t) \cos(3x)$ and the piecewise constant Galerkin basis $S = S_{-1,0}$. M is chosen so that $h^{3/2} \propto \Delta t^2$.

N	M	$\ \phi - \phi^{h,\lambda}\ _{-1/2,l^2}$	rate
4	22	0.66	-/-
8	40	0.26	1.34
16	68	0.082	1.67
32	116	0.023	1.84
64	204	0.0060	1.93
128	352	0.0015	1.99

Table 3: The results for scattering by the unit disk with $g(x, t) = \sin^5(t) \cos(3x)$ and the piecewise linear Galerkin basis $S = S_{0,1}$. M is chosen so that $h^{5/2} \propto \Delta t^2$.

$\theta \in [0, 2\pi)$. Since $\cos(l\theta)$ is an eigenfunction of the single layer potential $V(s_n)$, the Helmholtz problems can be solved exactly. However, to investigate the effect of spatial discretization we solve the problems using the Galerkin method and hence obtain an approximation $\phi^{h,\lambda}(t_n, \theta)$ of the unknown density. To investigate the error, we use the fact that $\phi(\theta, t) = \phi(t) \cos(l\theta)$ and solve with high accuracy for $\phi(t)$ by applying Lubich's method to the one dimensional problem (6.3). The error measure we use is the following:

$$\|\phi - \phi^{h,\lambda}\|_{-1/2,l^2} := \left(\sum_{n=0}^N \Delta t \|\phi(t_n) \cos(l\cdot) - \phi^{h,\lambda}(t_n, \cdot)\|_{H^{-1/2}(\Gamma)}^2 \right)^{1/2}.$$

The theory predicts the above error to be proportional to $h^{m+3/2} + \Delta t^2$, where $m = 0$ for the Galerkin basis of piecewise constant functions and $m = 1$ for the basis of piecewise linear functions. In all the experiments we choose λ as in (6.4). To see if the spatial discretization has introduced significant errors, we compute the error obtained when the Helmholtz problems are solved exactly. The results are given in the following table.

N	4	8	16	32	64	128
$\ \phi - \phi^{h,\lambda}\ _{-1/2,l^2}$	0.61	0.24	0.077	0.022	0.0057	0.0015

Comparing these results to Table 2 and Table 3 we see that the error due to the discretization in space is not significant.

N	$\#\mathbf{N}_z$	M	$\ \phi - \phi^{h,\lambda}\ _{-1/2,l^2}$	rate
4	3	24	2.9	-/-
8	5	40	2.9	-0.03
16	9	68	1.4	1.09
32	17	116	0.42	1.70
64	24	204	0.11	1.92
128	24	352	0.028	1.98
256	24	612	0.0072	1.99

Table 4: The results for scattering by the unit disk where the incoming wave is a Gaussian pulse and the piecewise linear Galerkin basis $S = S_{1,0}$ is used. The column $\#\mathbf{N}_z$ shows the number of Helmholtz problems actually solved.

6.3 Reduction of the number of systems

Let us now consider a signal that is smooth and of nearly limited time duration:

$$g(\mathbf{r}, t) = \cos(5t - \mathbf{r} \cdot \alpha) \exp(-1.5(5t - \mathbf{r} \cdot \alpha - 5)^2), \quad (6.5)$$

$\alpha = (1, 0)$. For such a Gaussian pulse our theory predicts that only $\mathcal{O}(N^\epsilon)$, for any fixed $\epsilon > 0$, Helmholtz systems need to be solved to obtain optimal convergence; see also Figure 2. The results for scattering by the unit disk and for piecewise-linear basis functions, $S = S_{1,0}$, are given in Table 4. Since we approximate by zero only the solutions of those Helmholtz problems whose right-hand sides are zero almost to machine precision, the number of Helmholtz problems, $\#\mathbf{N}_z$ is constant for large enough N . For this more complicated problem, for each N we have used the numerical solution using $2N$ steps in time and the corresponding number of nodes in the discretization in space as the reference solution.

7 Conclusion

We have described a method that requires the solution of a number of Helmholtz problems to obtain an approximate solution of the wave equation in an unbounded, homogeneous medium. We have proved stability and optimal convergence results for this approach. Further we have indicated ways in which to efficiently solve the resulting system of Helmholtz problems. The stability and convergence results of the perturbations introduced by the efficient solvers has also been presented.

The fast methods we propose to use are typically capable of computing a matrix-vector product in almost linear time, i.e., $\mathcal{O}(M \log^a M)$, of a single dense $M \times M$ system arising from the discretization of the Helmholtz single layer potential. In order to solve efficiently the linear system by an iterative method requiring only matrix-vector multiplication a good preconditioner is needed. The investigation of such preconditioner is beyond the scope of this paper. With a preconditioned iterative solver we expect to obtain computational costs which scale linearly, up to logarithmic terms, with respect to the number of unknowns NM . Important observation is that in some cases only a few Helmholtz systems need to be solved. Though this does not change the overall complexity (the discrete Fourier transformation still requires $\mathcal{O}(MN \log N)$ operations), it can hugely reduce the absolute time for the computation. The storage costs will also scale linearly since at any one time only a single linear

system representing the discretization of a Helmholtz problem needs to be stored. Since all the NM coefficients $\phi_{j,n}$ are stored, the storage costs are not better than linear. Crucially, since the Helmholtz problems to be solved are entirely decoupled, the proposed method is easily parallelizable.

These asymptotic estimates improve significantly both the storage and computational costs compared to the previously proposed approaches for the solution of the wave equation using the convolution quadrature discretization in time; see [23] and [21, 22, 27]. The asymptotic costs of the MOT method presented in [9, 17] are also almost linear in the number of degrees of freedom. Advantages of our method include the intrinsic parallel nature of the method, proven convergence and stability properties, and the relatively simple implementation details. In a forthcoming paper, algorithmic details for the data sparse approximations, a more in-depth asymptotic complexity analysis, and large scale computational results will be presented.

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