EXTENSIONS AND ANALYSIS OF AN ITERATIVE SOLUTION OF THE HELMHOLTZ EQUATION VIA THE WAVE EQUATION

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ABSTRACT. In this paper we extend analysis of the WaveHoltz iteration—a time-domain iterative method for the solution of the Helmholtz equation. We expand the previous analysis of energy conserving problems and prove convergence of the WaveHoltz iteration for problems with impedance boundary conditions in a single spatial dimension. We then consider interior Dirichlet/Neumann problems with damping in any spatial dimension, and show that for a sufficient level of damping the WaveHoltz iteration converges in a number of iteration independent of the frequency. Finally, we present a discrete analysis of the WaveHoltz iteration for a family of higher order time-stepping schemes. We show that the fixed-point of the discrete WaveHoltz iteration converges to the discrete Helmholtz solution with the order of the time-stepper chosen. We present numerical examples and demonstrate that it is possible to completely remove time discretization error from the WaveHoltz solution through careful analysis of the discrete iteration together with updated quadrature formulas.

1. INTRODUCTION

This is the second of a series of papers on time-domain methods for the numerical solution of the Helmholtz equation

\( \nabla \cdot (c^2(x) \nabla u) + \omega^2 u = f(x), \quad x \in \Omega, \)

for a domain \( \Omega \), frequency \( \omega \), and sound speed \( c(x) \). The Helmholtz equation (both acoustic and elastic) is useful for seismic, acoustic, and optics applications. The numerical solution of the Helmholtz equation is especially difficult due to the resolution requirements and the indefinite nature of the Helmholtz operator for large frequencies.

In the previous paper [5], we introduced a time-domain approach for solving the Helmholtz equation (1.1). Given the Helmholtz solution, \( u(x) \), the time-harmonic wave field \( \text{Re}\{u(x)e^{-i\omega t}\} \) satisfies the wave equation

\[
\begin{align*}
\frac{\partial^2 w}{\partial t^2} &= \nabla \cdot (c^2(x) \nabla w) - f(x) \cos(\omega t), \quad x \in \Omega, \quad 0 \leq t \leq T, \\
w(0, x) &= v_0(x), \quad w_t(0, x) = v_1(x),
\end{align*}
\]

2010 Mathematics Subject Classification. Primary 65M22, 65M12.

Key words and phrases. Wave equation, Helmholtz equation.

The first author is supported in part by STINT initiation grant IB2019–8154 and NSF Grant DMS-1913076. Any conclusions or recommendations expressed in this paper are those of the author and do not necessarily reflect the views of the NSF.

The second author is supported in part by STINT initiation grant IB2019–8154 and NSF Grant DMS-1913076. Any conclusions or recommendations expressed in this paper are those of the author and do not necessarily reflect the views of the NSF.

The third author is supported in part by STINT initiation grant IB2019–8154.
where $v_0 = \text{Re}\{u(x)\}$ and $v_1 = \omega \text{Im}\{u(x)\}$. In [5], we introduced an integral operator that time-filtered the wave solution resulting from initial data $v_0^n$, $v_1^n$. The time-filtering generates new iterates $v_0^{n+1}$, $v_1^{n+1}$ leading to a fixed-point iteration we named the WaveHoltz iteration. The convergence of the fixed-point iteration for interior problems with Dirichlet/Neumann boundary conditions (i.e. energy conserving problems) was proven in the continuous and discrete settings under a non-resonance condition. For such problems, the WaveHoltz iteration can be reformulated as a symmetric and positive-definite system which can be accelerated with Krylov subspace methods such as the conjugate gradient method and GMRES. Numerical experiments using the WaveHoltz iteration indicated promising scaling with frequency for problems also with outflow boundary conditions common in seismic applications, though no theoretical proof was given for the convergence of the method in that case.

In this paper, we extend the continuous and discrete analysis presented in the prequel. In [5], the continuous analysis was performed using a simplified iteration in which the initial velocity, $v_1^n$, is set to zero each iteration as solutions to the Helmholtz equation are real-valued. In this paper we begin by proving convergence of the WaveHoltz iteration without the assumption $v_1^n \equiv 0$. This result, together with appropriate extensions of the problem data, leads to a proof of convergence of the WaveHoltz iteration for problems with impedance boundary conditions in a single spatial dimension. To conclude the continuous analysis, we additionally consider the damped Helmholtz equation and prove that the iteration is convergent. Numerical results verify that for a sufficiently large damping, the number of iterations for the WaveHoltz iteration to reach convergence for damped Helmholtz equations is independent of frequency. We thus can guarantee convergence of the method to the Helmholtz solution via impedance conditions and/or damping, without any additional conditions, which we note is possible due to the absence of resonant frequencies.

For the discrete analysis, we investigate the effect of choice of time-stepper used for the WaveHoltz iteration. In [5], we noted that in the discrete case the WaveHoltz iteration converged to the solution of a discrete Helmholtz problem with modified frequency. We provided the modification for a centered second order time-stepping scheme which would recover the original discrete Helmholtz solution. Here we consider higher order modified equation (ME) time-stepping schemes, [30, 2], and show that the fixed-point of the discrete WaveHoltz iteration converges to the discrete Helmholtz solution with the order of the time-stepper chosen. We additionally show that, as in the case for EM-WaveHoltz [28], it is possible to completely remove time discretization error from the WaveHoltz solution through careful analysis of the discrete iteration and updated quadrature formulas.

The efficient solution of the Helmholtz equation (1.1) via iterative methods is notoriously difficult, especially for high-frequency problems of practical interest, and has been the subject of much research. We refer to our previous paper [5] for a more in-depth overview of the literature on techniques for solving the Helmholtz equation, as well as the review articles [14, 15, 11]. We focus on the literature that is closely related to the methods and approach used here.

The theoretical justification for working in the time-domain comes from the limiting amplitude principle, see [26, 23, 33]. The principle states that every solution to the wave equation with a time-harmonic forcing in the exterior of a domain
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with reflecting boundary conditions tends to the Helmholtz solution. Rather than evolving a wave equation forward in time to reach a steady state by appealing to the limiting amplitude principle, it is possible to cast the problem as a constrained convex least-squares minimization problem. This approach, originally proposed by Bristeau et al. [9], is the so-called Controllability Method (CM). The CM seeks to accelerate the convergence to the steady-state limit by minimizing the deviation from time-periodicity of the time-domain solution in second-order form.

In the original CM, along with later work by Heikkola et al. [20, 21], only scatterers with Dirichlet boundary conditions were considered as the original cost functional of [9] did not generally yield unique minimizers for other types of boundary conditions. An alternative functional, $J_\infty$, proposed by Bardos and Rauch in [7], however, did yield uniqueness of the minimizer at the cost of requiring the storage of the entire history of the computed solution to the wave equation which could be prohibitive for large problems.

For the wave equation in second-order form, the initial condition lies in $H^1 \times L^2$, requiring the solution of a coercive elliptic problem to find a Riesz representative for gradient calculations. Glowinski and Rossi [17] presented an update to the CM by considering the wave equation in first-order form, allowing the initial conditions to lie in a reflexive space and thus removing the need for an elliptic solve in each iteration. The discretization chosen in this case, however, had the drawback of requiring inversion of a mass-matrix at each time-step.

In more recent work by Grote and Tang, [19], the use of an alternative functional (or post-processing via a compatibility condition) restored uniqueness of the minimizer of CM. In a follow-up paper, [25], Grote et al. proposed the use of a hybrid discontinuous Galerkin discretization, [31], of the first-order form wave equation which allowed the scheme to be fully explicit and therefore fully parallel. Moreover, they extend CM to general boundary conditions for the first-order formulation and additionally proposed a filtering procedure which allows the original energy functional to be used regardless of the boundary condition.

The above work has inspired other time-domain methods outside of CM and WaveHoltz. Work by Stolk [32] utilizes time-domain approaches as a preconditioner for a GMRES accelerated preconditioner for direct Helmholtz discretizations yielding a hybrid time-frequency domain method. Arnold et al. [6] propose a time-domain method for scattering problems which leverages the compact support of incident field plane wavelets together with a front-tracking adaptive meshing algorithm to reduce the cost of computing a Fourier transform of the wave solution to obtain Helmholtz solutions.

Another important class of methods for solving the Helmholtz equation are the so-called shifted Laplacian preconditioners. The use of the Laplacian as a preconditioner for Helmholtz problems emerged with the initial work of Bayliss et al. [8]. In [8], the normal equations of the discrete Helmholtz equation were iteratively solved using conjugate gradient, with a Symmetric Successive Over-Relaxation (SSOR) sweep of the discrete Laplacian as a preconditioner. Giles and Laird then extended the previous preconditioner to instead solve the Helmholtz system with a flipped sign in front of the Helmholtz term using multigrid [24]. Erlangga, Vuij and Oosterlee [13, 10] further generalized the previous work to use a complex-valued shift of the Laplacian leading to the shifted Laplacian preconditioner. For a review of the
class of shifted Laplacian preconditioners we refer the reader to the review article by Erlangga [11].

The rest of this paper is organized as follows. In Section 2 we present analysis for the general WaveHoltz iteration and prove convergence in the case of impedance boundary conditions in a single spatial dimension. In Section 3 we present a brief analysis for the case in which damping is present. Section 4 outlines a discrete analysis of higher order modified equation (ME) schemes, and we additionally present a method to completely remove time discretization error from the discrete WaveHoltz solution. Finally, in Section 5 we describe our numerical methods, Section 6 present our numerical examples, and summarize the paper in Section 7.

2. The General Iteration

We consider the Helmholtz equation in a bounded open smooth domain $\Omega$,

\begin{equation}
\nabla \cdot (c^2(x) \nabla u) + \omega^2 u = f(x), \quad x \in \Omega,
\end{equation}

with boundary conditions of the type

\begin{equation}
i\alpha u + \beta(c(x)\vec{n} \cdot \nabla u) = 0, \quad \alpha^2 + \beta^2 = 1, \quad x \in \partial \Omega.
\end{equation}

We assume $f \in L^2(\Omega)$ and that $c \in L^\infty(\Omega)$ with the bounds $0 < c_{\min} \leq c(x) \leq c_{\max} < \infty$ a.e. in $\Omega$. Away from resonances, this ensures that there is a unique weak solution $u \in H^1(\Omega)$ to (2.1). Due to the boundary conditions $u$ is in general complex-valued.

We first note that the function $w(t,x) := \text{Re}\{u(x)\exp(-i\omega t)\}$ is a $T = 2\pi/\omega$-periodic (in time) solution to the real-valued forced scalar wave equation

\begin{equation}
w_{tt} = \nabla \cdot (c^2(x) \nabla w) - \text{Re}\{f(x)e^{-i\omega t}\}, \quad x \in \Omega, \quad 0 \leq t \leq T,
\end{equation}

\begin{equation}
w(0,x) = v_0(x), \quad w_t(0,x) = v_1(x),
\end{equation}

where $v_0 = \text{Re}\{u\}$ and $v_1 = \omega \text{Im}\{u\}$. Based on this observation, our approach is to find this $w$ instead of $u$. We could thus look for initial data $v_0$ and $v_1$ such that $w$ is a $T$-periodic solution to (2.3). However, there may be several such $w$, see [19], and we therefore impose the alternative constraint that a certain time-average of $w$ should equal the initial data. More precisely, we introduce the following operator acting on the initial data $v_0 \in H^1(\Omega)$, $v_1 \in L^2(\Omega)$,

\begin{equation}
\Pi \left[ \begin{array}{c} v_0 \\ v_1 \end{array} \right] = \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) \left[ \begin{array}{c} w(t,x) \\ w_t(t,x) \end{array} \right] dt, \quad T = \frac{2\pi}{\omega},
\end{equation}

where $w(t,x)$ and its time derivative $w_t(t,x)$ satisfies the wave equation (2.3) with initial data $v_0$ and $v_1$. The result of $\Pi[v_0, v_1]^T$ can thus be seen as a filtering in time of $w(\cdot, x)$ around the $\omega$-frequency. By construction, the solution $u$ of Helmholtz now satisfies the system of equations

\begin{equation}
\left[ \begin{array}{c} \text{Re}\{u\} \\ \omega \text{Im}\{u\} \end{array} \right] = \Pi \left[ \begin{array}{c} \text{Re}\{u\} \\ \omega \text{Im}\{u\} \end{array} \right].
\end{equation}

The WaveHoltz iteration then amounts to solving this system of equations with the fixed point iteration

\begin{equation}
\left[ \begin{array}{c} v \\ v' \end{array} \right]^{(n+1)} = \Pi \left[ \begin{array}{c} v \\ v' \end{array} \right]^{(n)}, \quad \left[ \begin{array}{c} v \\ v' \end{array} \right]^{(0)} = 0.
\end{equation}
Provided this iteration converges and the solution to is unique, we obtain the Helmholtz solution as \( u = \lim_{n \to \infty} v^n \).

As seen in [5], the WaveHoltz operator \( \Pi \) is affine and can be written as \( \Pi v = S v + b \), where \( S \) is a linear operator, \( v = (v, v')^T \) and \( b \) a fixed function. Since the sought solution satisfies \( \Pi v = v \), we can then reformulate the iteration as a linear system

\[
Av = b, \quad A = I - S,
\]

which allows the convergence of the WaveHoltz iteration to be accelerated by a Krylov method. We note that the right hand side can be computed by applying the WaveHoltz operator to the zero function, \( b = \Pi 0 \). The action of \( A \) can also be computed via one application of \( \Pi \), as \( Av = v - \Pi v + b \). Hence, after precomputing \( b \) the action can be computed by applying \( \Pi \) to \( v \), i.e. by evolving the wave equation for one period in time with initial data \( v \) and filter the solution. There is no need to explicitly form \( A \).

**Remark 2.1.** The operator \( A \) for the general iteration is not symmetric unlike the simplified iteration for energy conserving problems where \( v_1 = 0 \). For interior, energy conserving problems we recommend the use of the simplified iteration so that the conjugate gradient method may be used to accelerate convergence. For other boundary conditions, the general WaveHoltz iteration is required and a more versatile Krylov method, such as GMRES, should be used.

### 2.1. Convergence for the Energy Conserving Case for the General WaveHoltz Iteration.

Here we consider boundary conditions of either Dirichlet (\( \beta = 0 \)) or Neumann (\( \alpha = 0 \)) type in (2.3). This is typically the most difficult case for iterative Helmholtz solvers when \( \Omega \) is bounded. The wave energy is preserved in time and certain \( \omega \)-frequencies in Helmholtz are resonant, meaning they equal an eigenvalue of the operator \( -\nabla \cdot (c^2(x)\nabla) \). Moreover, the limiting amplitude principle does not hold, and one can thus not obtain the Helmholtz solution by solving the wave equation over a long time interval. We note that convergence of the WaveHoltz iteration in the energy conserving case was proved in [5] using a simplified iteration for which \( v'^{(n)} \equiv 0 \) in (2.6). In this section we prove convergence of the general iteration (2.6) without the assumption that \( v'^{(n)} \equiv 0 \). With this result in hand, it will then be possible to establish convergence for the non-energy conserving case in Section 2.2.

By the choice of boundary conditions the operator \( -\nabla \cdot (c^2(x)\nabla) \) has a point spectrum with non-negative eigenvalues. Denote those eigenmodes \( (\lambda_j^2, \phi_j(x)) \). We assume that the angular frequency \( \omega \) is not a resonance, i.e. \( \omega^2 \neq \lambda_j^2 \) for all \( j \). The Helmholtz equation (1.1) is then wellposed.

We recall that for any \( q \in L^2(\Omega) \) we can expand

\[
q(x) = \sum_{j=0}^{\infty} q_j \phi_j(x),
\]

for some coefficients \( q_j \) and

\[
\|q\|_{L^2(\Omega)}^2 = \sum_{j=0}^{\infty} |q_j|^2, \quad c_{\min}^2 \|\nabla q\|_{L^2(\Omega)}^2 \leq \sum_{j=0}^{\infty} \lambda_j^2 |q_j|^2 \leq c_{\max}^2 \|\nabla q\|_{L^2(\Omega)}^2.
\]
We start by expanding the Helmholtz solution $u = u^R + iu^I$, the initial data $v_0, v_1$ to the wave equation (2.3), and the forcing $f = f^R + if^I$ in this way,

$$u^R(x) = \sum_{j=0}^{\infty} u^R_j \phi_j(x), \quad v_0(x) = \sum_{j=0}^{\infty} v_{0,j} \phi_j(x),$$

$$v_1(x) = \sum_{j=0}^{\infty} v_{1,j} \phi_j(x), \quad f^R(x) = \sum_{j=0}^{\infty} f^R_j \phi_j(x),$$

with analogous expansions for the imaginary parts of $u$ and $f$, $u^I$ and $f^I$, respectively. Then,

$$-\lambda_j^2 u^R_j + \omega^2 u^R_j = f^R_j \Rightarrow u^R_j = \frac{f^R_j}{\omega^2 - \lambda_j^2},$$

and similarly for the imaginary parts $u^I_j$ and $f^I_j$. For the wave equation solution $w(t, x)$ with initial data $w = v_0$ and $w_t = v_1$ we have

$$w(t, x) = \sum_{j=0}^{\infty} w_j(t) \phi_j(x),$$

where

$$w_j(t) = u^R_j \left[ \cos(\omega t) - \cos(\lambda_j t) \right] + u^I_j \left[ \sin(\omega t) - \frac{\omega}{\lambda_j} \sin(\lambda_j t) \right] + v_{0,j} \cos(\lambda_j t) + \frac{v_{1,j}}{\lambda_j} \sin(\lambda_j t),$$

with

$$w^0_{\text{Neu}}(t) = u^R_0 \left[ \cos(\omega t) - 1 \right] + u^I_0 \left[ \sin(\omega t) - \omega t \right] + v_{0,0} + v_{1,0} t,$$

if $\lambda_0 = 0$, as is the case for Neumann boundary conditions (a special case which we denote via the superscript ‘Neu’ in the following analysis). The filtering step then gives

$$\Pi \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \sum_{j=0}^{\infty} \begin{bmatrix} \bar{v}_j \\ \bar{\bar{v}}_j \end{bmatrix} \phi_j(x),$$

where

$$\bar{v}_j = u^R_j (1 - \beta(\lambda_j)) - u^I_j \frac{\omega}{\lambda_j} \gamma(\lambda_j) + v_{0,j} \beta(\lambda_j) + \frac{v_{1,j}}{\lambda_j} \gamma(\lambda_j),$$

$$\bar{\bar{v}}_j = u^R_j \lambda_j \gamma(\lambda_j) + \omega u^I_j (1 - \beta(\lambda_j)) - v_{0,j} \lambda_j \gamma(\lambda_j) + v_{1,j} \beta(\lambda_j),$$

and

$$\beta(\lambda) := \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) \cos(\lambda t) dt, \quad \gamma(\lambda) := \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) \sin(\lambda t) dt.$$

When $\lambda_j \neq 0$. For the Neumann case, we have

$$\bar{v}_0 = \frac{3}{2} u^R_0 + \frac{\pi}{2} u^I_0 - \frac{1}{2} v_{0,0} - \frac{\pi}{2\omega} v_{1,0}, \quad \bar{\bar{v}}_0 = \frac{3}{2} u^R_0 - \frac{1}{2} v_{1,0}.$$

By definition we have

$$\left| \frac{\gamma(\lambda_j)}{\lambda_j} \right| \leq \frac{2}{T} \int_0^T \left| \left( \cos(\omega t) - \frac{1}{4} \right) t \frac{\sin(\lambda t)}{\lambda t} \right| dt \leq \frac{2}{T} \int_0^T \frac{5}{4} t dt = \frac{5\pi}{2\omega},$$

for all $\lambda_j$. 

(2.7)
since \(|\sin(x)/x| \leq 1\), which ensures the boundedness of the coefficients \(v_j, \bar{v}_j\) for small eigenvalues \(\lambda_j\).

Letting \(v_{0,j}, v_{1,j}\) denote the coefficients of \(v_0, v_1\) in the eigenbasis of the Laplacian, we can write the iteration as

\[
\begin{bmatrix}
  v_{0,j}^{n+1} \\
  v_{1,j}^{n+1}
\end{bmatrix} = \left( \Pi \begin{bmatrix} v_0^n \\ v_1^n \end{bmatrix} \right)_j = (I - B_j) \begin{bmatrix} u_j^R \\ \omega u_j^I \end{bmatrix} + B_j \begin{bmatrix} v_{0,j}^n \\ v_{1,j}^n \end{bmatrix},
\]

where if we define \(\beta_j = \beta(\lambda_j)\) and \(\gamma_j = \gamma(\lambda_j)\) then

\[
B_j = \begin{pmatrix} \beta_j & \gamma_j/\lambda_j \\ -\lambda_j \gamma_j & \beta_j \end{pmatrix}, \quad B_0^{\text{Neu}} = \begin{pmatrix} -1/2 & -\pi/2\omega \\ 0 & -1/2 \end{pmatrix},
\]

Moreover, the eigenvectors and eigenvalues of \(B_j\) are

\[
\xi_j^\pm = \left( \pm i/\lambda \atop 1 \right), \quad \xi_0^{\text{Neu}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mu_j = \beta_j \pm i\gamma_j.
\]

Introducing the linear operator \(S : L^2(\Omega) \times L^2(\Omega) \to L^2(\Omega) \times L^2(\Omega)\),

\[
S \sum_{j=0}^\infty \begin{bmatrix} u_j^R \\ u_j^I \end{bmatrix} \phi_j(x) = \sum_{j=0}^\infty B_j \begin{bmatrix} u_j^R \\ u_j^I \end{bmatrix} \phi_j(x),
\]

we may write the iteration as

\[
\left( \begin{bmatrix} v \\ v' \end{bmatrix} \right)^{(n+1)} = \Pi \left( \begin{bmatrix} v \\ v' \end{bmatrix} \right)^{(n)} = \left[ \begin{bmatrix} u_j^R \\ \omega u_j^I \end{bmatrix} \right] + S \left( \left[ \begin{bmatrix} v \\ v' \end{bmatrix} \right]^{(n)} - \left[ \begin{bmatrix} u_j^R \\ \omega u_j^I \end{bmatrix} \right] \right).
\]

We note that, in contrast to the simplified iteration analyzed in [5], the operator \(S\) is not symmetric for the general iteration. Despite this, we may identify the eigenmodes of \(S\) from the eigenvectors of \(B_j\) via \(\xi_j^\pm \phi_j\) with eigenvalues \(\mu_j = \beta_j \pm i\gamma_j\) and \(\xi_0^{\text{Neu}} = \xi_0^{\text{Neu}} \phi_0\) with eigenvalue \(\mu_0^{\text{Neu}} = -1/2\).

From (2.8), we see that the iteration for each mode takes the form

\[
\begin{bmatrix} v_{0,j}^{n+1} \\ v_{1,j}^{n+1} \end{bmatrix} = \left( \Pi \begin{bmatrix} v_0^n \\ v_1^n \end{bmatrix} \right)_j = (I - B_j^n) \begin{bmatrix} u_j^R \\ \omega u_j^I \end{bmatrix} + B_j^n \begin{bmatrix} v_{0,j}^n \\ v_{1,j}^n \end{bmatrix},
\]

so that

\[
\begin{bmatrix} v_{0,j}^{n+1} - u_j^R \\ v_{1,j}^{n+1} - \omega u_j^I \end{bmatrix} = B_j^n \begin{bmatrix} v_{0,j}^n - u_j^R \\ v_{1,j}^n - \omega u_j^I \end{bmatrix}.
\]

We thus require that \(B_j^n \to 0\) uniformly in \(j\) to ensure convergence of the fixed-point iteration to the solution, \([u_j^R, \omega u_j^I]^T\), which is true if and only if the spectral radius of \(B_j\) is less than unity uniformly in \(j\). That is, we require that \(|\mu_j| < 1\) uniformly in \(j\). Defining the filter function \(\mu(\lambda) := \beta(\lambda) + i\gamma(\lambda)\), we may show (with a proof in Appendix A) the following lemma

**Lemma 2.2.** The complex-valued filter function \(\mu\) satisfies \(\mu(\omega) = 1\) and

\[
0 \leq |\mu(\lambda)| \leq 1 - \frac{15}{32} \left( \frac{\lambda - \omega}{\omega} \right)^2, \quad \text{when} \quad \left| \frac{\lambda - \omega}{\omega} \right| \leq \frac{1}{2},
\]

\[
|\mu(\lambda)| \leq \frac{7}{3\pi} \approx 0.74, \quad \text{when} \quad \left| \frac{\lambda - \omega}{\omega} \right| \geq \frac{1}{2},
\]

\[
|\mu(\lambda)| \leq b_0 \frac{\omega}{|\lambda - \omega|}, \quad \text{when} \quad \lambda > \omega,
\]
where \( b_0 = 3/2\pi \). Moreover, close to \( \omega \) we have the local expansion

\[
|\mu(\omega + r)| = 1 - b_1 \left( \frac{r}{\omega} \right)^2 + R(r/\omega) \left( \frac{r}{\omega} \right)^3,
\]

\[
b_1 = \frac{\pi^2}{6} - \frac{1}{4} \approx 1.39, \quad ||R||_{\infty} \leq \frac{25\pi^4}{4} (36 + 20\pi + 25\pi^2 + 75\pi^3).
\]

We denote

\[
\delta_j = \frac{\lambda_j - \omega}{\omega},
\]

the relative size of the gap between \( \lambda_j \) and the Helmholtz frequency, and then denote the smallest gap (in magnitude) by \( \delta \),

\[
\delta = \delta_j^*, \quad j^* = \text{argmin}_j |\delta_j|.
\]

Then we have the following lemma

**Lemma 2.3.** Suppose \( \delta > 0 \). Then, the spectral radius \( \rho \) of \( S \) is strictly less than one, and for small \( \delta \),

\[
\rho = 1 - b_1 \delta^2 + O(\delta^3),
\]

with \( b_1 \) as in Lemma 2.2. Moreover, \( S \) is a bounded linear map from \( L^2(\Omega) \times L^2(\Omega) \) to \( H^1(\Omega) \times L^2(\Omega) \), and from \( H^1(\Omega) \times L^2(\Omega) \) to \( H^1(\Omega) \times H^1(\Omega) \).

**Proof.** Let \( a_0 = 15/32 \), \( a_1 = 7/3\pi \) and \( a_2 = \sqrt{(1 - a_1)/a_0}/2 \approx 0.74 \). From Lemma 2.2 we get

\[
\rho = \sup_j |\mu(\lambda_j)| \leq \sup_j \max \left( 1 - a_0 \delta_j^2, \ a_1 \right) \leq \max \left( 1 - a_0 \delta_j^2, \ a_1 \right) < 1.
\]

For the more precise estimate when \( \delta \) is small we will use (2.12). Since \( 1 > \rho \geq |\mu(\omega + \omega \delta)| \to 1 \) as \( \delta \to 0 \), we can assume that \( \rho > 1 - a_0 \eta^2 \), with \( \eta := \min(b_1/2||R||_{\infty}, \ a_2) \), for small enough \( \delta \). Then, for \( |\delta_j| > \eta \) we have \( |\mu(\omega + \omega \delta_j)| \leq \max(1 - a_0 \eta^2/2, \ a_1) = 1 - a_0 \eta^2/2 \). Consequently, by Lemma 2.2, we have

\[
\rho = \max_{|\delta_j| \leq \eta} |\mu(\omega + \omega \delta_j)| = |\mu(\omega + \omega \delta_{j^*})|,
\]

for some \( k^* \) with \( |\delta_{k^*}| \leq \eta \). If \( \delta_{k^*} = \delta_{j^*} \) (where \( \delta = |\delta_j| \)) then (2.12) gives (2.13).

If not, we have \( \eta \geq |\delta_{k^*}| \geq \delta \) and by Lemma 2.2

\[
0 \leq |\mu(\omega + \omega \delta_{k^*})| - |\mu(\omega + \omega \delta_{j^*})| = -b_1 (\delta_{k^*}^2 - \delta^2) + R(\delta_{k^*}) \delta_{k^*}^3 - R(\delta_{j^*}) \delta_{j^*}^3, = -b_1 (\delta_{k^*}^2 - \delta^2) + \frac{b_1}{2} (\delta_{k^*}^2 + \delta^2),
\]

which implies that \( \delta_{k^*}^2 \leq 3 \delta^2 \) and \( \delta^2 - \delta_{k^*}^2 = O(\delta^3) \). Therefore

\[
\rho = 1 - b_1 \delta_{k^*}^2 + O(\delta_{k^*}^3) = 1 - b_1 \delta^2 + b_1 (\delta^2 - \delta_{k^*}^2) + O(\delta_{k^*}^3) = 1 - b_1 \delta^2 + O(\delta_{k^*}^3 + \delta^3) = 1 - b_1 \delta^2 + O(\delta^3),
\]

from which (2.13) follows.

Letting \( D := \omega \min(1, b_0(1 + 1/|\delta|)) \), we note that by Lemma 2.2,

\[
|\lambda_j \mu(\lambda_j)| \leq \omega \leq D, \quad \lambda_j \leq \omega,
\]

\[
|\lambda_j \mu(\lambda_j)| \leq \omega \frac{b_0 \lambda_j}{\lambda_j - \omega} = \omega b_0(1 + 1/\delta_j) \leq D, \quad \lambda_j > \omega.
\]
Moreover, the triangle inequality gives that $|\beta(\lambda_j)|, |\gamma(\lambda_j)| \leq |\mu(\lambda_j)|$, which implies both $\lambda_j|\beta(\lambda_j)| \leq D$ and $\lambda_j|\gamma(\lambda_j)| \leq D$.

Suppose now that $g, h \in L^2(\Omega)$ and

$$g(x) = \sum_{j=0}^{\infty} g_j \phi_j(x), \quad h(x) = \sum_{j=0}^{\infty} h_j \phi_j(x).$$

Let $z = [g, h]^T$ and define $C := \max\{D, |\gamma(\lambda_j)|/\lambda_j, \pi/2\omega\}$, which is bounded for $\lambda_j \neq 0$ via the estimate (2.7). Then straightforward algebra gives the bound

$$||S||_{L^2(\Omega) \times L^2(\Omega)}^2 = \sum_{j=0}^{\infty} \left| \begin{bmatrix} g_j \\ h_j \end{bmatrix} \right|^2$$

$$= \sum_{j=0}^{\infty} \left| \beta(\lambda_j)g_j + \frac{\gamma(\lambda_j)}{\lambda_j} h_j \right|^2 + |\lambda_j\gamma(\lambda_j)g_j - \beta(\lambda_j)h_j|^2$$

$$\leq \sum_{j=0}^{\infty} (1 + C^2)(|g_j|^2 + |h_j|^2) + 4C|g_j||h_j|$$

$$\leq (1 + C^2 + 2C)||z||_{L^2(\Omega) \times L^2(\Omega)}^2,$$

since $2|ab| \leq a^2 + b^2$. In the case of Neumann boundary conditions we have $\lambda_0 = 0$ and and the zeroth term must be treated specially. Using $B_{0, \text{Neu}}$ we get the same estimate

$$\left\| B_{0, \text{Neu}} \begin{bmatrix} g_0 \\ h_0 \end{bmatrix} \right\|^2 = \frac{1}{2} g_0 \left( \frac{\pi}{2\omega} h_0 \right)^2 + \frac{1}{4} |h_0|^2$$

$$\leq \frac{1}{4} |g_0|^2 + \frac{\pi}{2 \omega} |g_0||h_0| + \frac{\pi^2}{4 \omega^2} |h_0|^2 + \frac{1}{4} |h_0|^2$$

$$\leq \left( \frac{1}{4} + \frac{1}{2} C \right)(|g_0|^2 + |h_0|^2) + C^2 |h_0|^2$$

$$\leq (1 + 2C + C^2)(|g_0|^2 + |h_0|^2),$$

so that in conclusion $||S||_{L^2(\Omega) \times L^2(\Omega)}^2 \leq (1 + C^2 + 2C)||z||_{L^2(\Omega) \times L^2(\Omega)}^2$ for both cases.

Next we let $S = [\bar{g}, \bar{h}]^T$. Then, if $g, h \in L^2(\Omega)$,

$$||\nabla \bar{g}||_{L^2(\Omega)}^2 \leq \sum_{j=0}^{\infty} \frac{\lambda_j^2}{c^2_{\min}} \left| \beta(\lambda_j)g_j + \frac{\gamma(\lambda_j)}{\lambda_j} h_j \right|^2 \leq \sum_{j=0}^{\infty} \frac{2(D^2 + 1)}{c^2_{\min}} \left( |\lambda_j\beta(\lambda_j)g_j|^2 + |\gamma(\lambda_j)h_j|^2 \right)$$

$$\leq \sum_{j=0}^{\infty} \frac{2(D^2 + 1)}{c^2_{\min}} \left( |g_j|^2 + |h_j|^2 \right) = \frac{2(D^2 + 1)}{c^2_{\min}} ||\nabla \bar{g}||_{L^2(\Omega)}^2,$$

which gives

$$||S||_{H^1(\Omega) \times L^2(\Omega)} = ||S||_{L^2(\Omega) \times L^2(\Omega)} + ||\nabla \bar{g}||_{L^2(\Omega)}^2$$

$$\leq \left( 1 + C^2 + 2C + \frac{2(D^2 + 1)}{c^2_{\min}} \right) ||\nabla \bar{g}||_{L^2(\Omega) \times L^2(\Omega)}^2,$$

showing that $S$ is a bounded linear map from $L^2(\Omega) \times L^2(\Omega)$ to $H^1(\Omega) \times L^2(\Omega)$. 

If instead $g \in H^1(\Omega)$ and $h \in L^2(\Omega)$, we compute

$$||\nabla \tilde{h}||_{L^2(\Omega)}^2 \leq \sum_{j=0}^{\infty} \frac{\lambda_j^2}{c_{\min}^2} \left| -\gamma(\lambda_j)\lambda_j g_j + \beta(\lambda_j)h_j \right|^2$$

\[
\leq \sum_{j=0}^{\infty} \frac{2}{c_{\min}^2} \left( |\gamma(\lambda_j)\lambda_j g_j|^2 + |\beta(\lambda_j)\lambda_j h_j|^2 \right)
\]

\[
\leq \frac{2D^2}{c_{\min}} \sum_{j=0}^{\infty} (\lambda_j^2|g_j|^2 + |h_j|^2)
\]

\[
\leq \frac{2D^2}{c_{\min}} \left( c_{\max}^2 ||\nabla g||_{L^2(\Omega)}^2 + ||h||_{L^2(\Omega)}^2 \right) \leq \frac{2D^2(c_{\max}^2 + 1)}{c_{\min}^2} ||z||_{H^1(\Omega) \times L^2(\Omega)}^2
\]

so that

$$||Sz||_{H^1(\Omega) \times L^1(\Omega)} = ||Sz||_{H^1(\Omega) \times L^2(\Omega)} + ||\nabla \tilde{h}||_{L^2(\Omega)}^2 \leq \left( 1 + C^2 + 2C + \frac{2D^2(c_{\max}^2 + 2) + 2}{c_{\min}^2} \right) ||z||_{H^1(\Omega) \times L^2(\Omega)}^2$$

which shows that $S$ is a bounded linear map from $H^1(\Omega) \times L^2(\Omega)$ to $H^1(\Omega) \times H^1(\Omega)$, concluding the proof of the lemma.

Further, denoting $e^n := [\text{Re}\{u\} - v_0^n, \omega \text{Im}\{u\} - v_1^n]^T = [v_0^n, v_1^n]^T$, from (2.10) we obtain

$$e^n = S[\text{Re}\{u\} - v_0^{n-1}, \omega \text{Im}\{u\} - v_1^{n-1}]^T = Se^{n-1} = S^ne^0,$$

which shows that $e^n \to 0$ since $S^n \to 0$. Thus the iterates $[v_0^n, v_1^n]^T$ converge to $[\text{Re}\{u\}, \omega \text{Im}\{u\}]^T$ in $L^2(\Omega) \times L^2(\Omega)$. Since $v_0^0 = v_1^0 = 0$, it follows from Lemma 2.3 that the iterates $[v_0^n, v_1^n]^T$ and $[v_0^n, e_1^n]^T$ both belong to $H^1(\Omega) \times H^1(\Omega)$ for $n > 0$ when $u \in H^2(\Omega)$, as $S$ is a bounded linear map from $H^1(\Omega) \times L^2(\Omega)$ to $H^1(\Omega) \times H^1(\Omega)$. We can therefore also get convergence in $H^1(\Omega) \times H^1(\Omega)$. To show this, let

$$\beta_j + i\gamma_j = r_j \exp(i\phi_j), \quad r_j^2 = |\beta_j|^2 + |\gamma_j|^2, \quad \phi_j = \arctan(\gamma_j/\beta_j).$$

It can then be shown that powers of the operator $B_j$ can be written as

$$B_j^n = r_j^n \begin{pmatrix} \cos(n\phi_j) & \sin(n\phi_j)/\lambda_j \\ -\lambda_j \sin(n\phi_j) & \cos(n\phi_j) \end{pmatrix}.$$
We conclude that the iteration converges in $H^1(\Omega)$ where each entry is bounded and goes to zero in the limit as $n \to \infty$ since the spectral radius of $B_j$ is less than one. Then, using the fact that $|r_j\lambda_j| \leq D$, 

$$\|\nabla e^n\|_{L^2(\Omega)}^2 = \|\nabla S^n e^n\|_{L^2(\Omega)}^2 \leq \sum_{j=0}^{\infty} \lambda_j^2 r_j^{2n} e_{j,0}^2 \left| \frac{\cos(n\phi_j) e_{j,0}}{\lambda_j} + \frac{\sin(n\phi_j)}{\lambda_j} e_{j,1}^2 \right|^2$$

$$\leq \sum_{j=0}^{\infty} \frac{2n^2 \lambda_j^2 r_j^{2n}}{\min \lambda_j^2} \left( \lambda_j^2 |e_{j,0}|^2 + |e_{j,1}|^2 \right) + \frac{2n^2 \lambda_j^2 r_j^{2n}}{\min \lambda_j^2} \left( \lambda_j^2 |e_{j,0}|^2 + |e_{j,1}|^2 \right)$$

$$\leq \left( \sup r_j \right)^{2n-2} \frac{2(1+D^2)}{\min \lambda_j^2} \sum_{j=0}^{\infty} \lambda_j^2 |e_{j,0}|^2 + |e_{j,1}|^2$$

$$\leq \rho^{2n-2} \frac{2(1+D^2)}{\min \lambda_j^2} \left( c_{\max}^2 \|\nabla e^n\|_{L^2(\Omega)}^2 + \|e^n\|_{L^2(\Omega)}^2 \right) \to 0.$$ 

We conclude that the iteration converges in $H^1(\Omega) \times H^1(\Omega)$ with convergence rate $\rho$. By Lemma 2.3 we have $\rho \approx 1 - 1.39\delta^2$ so that the smallest gap, $\delta$, determines the convergence rate. We thus have proven the following theorem.

**Theorem 2.4.** Suppose $u \in H^1(\Omega)$ is the solution of the Helmholtz equation (1.1). The iteration in (2.6) and (2.4) converges in $H^1(\Omega) \times H^1(\Omega)$ for the Dirichlet and Neumann problems away from resonances to $[\text{Re}\{u\}, \text{Im}\{u\}]^T$. The convergence rate is $1 - O(\delta^2)$, where $\delta$ is the minimum gap between $\omega$ and the eigenvalues of $-\nabla \cdot (c^2(x)\nabla)$.

### 2.2. Convergence in the Non-Energy Conserving Case

With Theorem 2.4 providing convergence of the general WaveHoltz iteration in the energy conserving case, we turn toward proving convergence for problems with impedance boundary conditions. For simplicity we prove convergence in a single spatial dimension. We note that it is possible to use the following approach to prove convergence for certain problems in higher dimensions, e.g. problems with a constant wavespeed in certain simple geometries. Consider now the following Helmholtz problem with impedance boundary conditions

$$\frac{\partial}{\partial x} \left[ c^2(x) \frac{\partial}{\partial x} u(x) \right] + \omega^2 u(x) = f(x), \quad a \leq x \leq b,$$

(2.14)  

$$i\alpha u(a) - \beta c(x) u_x(a) = 0,$$

$$i\alpha u(b) + \beta c(x) u_x(b) = 0,$$

where $\alpha^2 + \beta^2 = 1$, but $\alpha, \beta \neq 0$. As before we assume that $c \in L^\infty(a, b)$ with the bounds $0 < c_{\min} \leq c(x) \leq c_{\max} < \infty$ a.e. in $(a, b)$, and $f \in L^2(a, b)$, but we now require additionally that $f$ is compactly supported in $(a, b)$ and that $c(a) = c_a, c(b) = c_b$ with $c$ constant in a neighborhood of the endpoints. We reformulate this
in the time domain as
\[ w_{tt} = \frac{\partial}{\partial x} \left[ c^2(x) \frac{\partial}{\partial x} w \right] - f(x) e^{-i\omega t}, \quad a \leq x \leq b, \quad 0 \leq t \leq T, \]
\[ w(0, x) = v_0(x), \quad w_t(0, x) = v_1(x), \]
\[ \alpha w_t(t, a) - \beta c(x) w_x(t, a) = 0, \]
\[ \alpha w_t(t, b) + \beta c(x) w_x(t, b) = 0. \]

In general, the solution of the above equation will yield complex-valued solutions and so we take the real part of the equation as shown earlier and use the general iteration (2.6). Note that in 1D the impedance boundary conditions with \( \alpha = \beta = 1/\sqrt{2} \) are equivalent to outflow/radiation conditions when the initial data is compactly supported in the interval \([a, b] \). If \( \alpha \neq \beta \) with \( \alpha, \beta \neq 0 \), then in addition to outgoing waves at the boundary there will be reflections due to the impedance boundary condition. In either case, if we let \( \tilde{a} < a - c_0 T/2 \) and \( \tilde{b} > b + c_0 T/2 \), then \( w \) is equal to \( \tilde{w} \) on \([a, b] \) for \( t \in [0, T] \) if \( \tilde{w} \) solves the following Neumann problem in the extended domain \( \tilde{\Omega} := [\tilde{a}, \tilde{b}] \supset [a, b] := \Omega \)
\[ \tilde{w}_{tt} = \frac{\partial}{\partial x} \left[ c^2(x) \frac{\partial}{\partial x} \tilde{w} \right] - \text{Re}\{\hat{f}(x) e^{-i\omega t}\}, \quad \tilde{a} \leq x \leq \tilde{b}, \quad 0 \leq t \leq T, \]
(2.15) \[ \tilde{w}(0, x) = \tilde{v}_0(x), \quad \tilde{w}_t(0, x) = \tilde{v}_1(x), \]
\[ \tilde{w}_x(t, \tilde{a}) = 0, \quad \tilde{w}_x(t, \tilde{b}) = 0, \]

where \( \tilde{v}_0 \) and \( \tilde{c} \) are the constant extensions (with \( \gamma = \alpha/\beta \))
\[ \tilde{v}_0(x) = \begin{cases} v_0(a), & \tilde{a} \leq x < a, \\ v_0(x), & a \leq x \leq \tilde{b}, \\ \tilde{c}(x), & \tilde{b} < x \leq b, \end{cases} \]
and \( \tilde{v}_1, \tilde{f} \) are zero extensions of \( v_1 \) and \( f \),
\[ \tilde{v}_1(x) = \begin{cases} 0, & \tilde{a} \leq x < a, \\ v_1(x), & a \leq x \leq \tilde{b}, \\ 0, & \tilde{b} < x \leq b, \end{cases} \]
\[ \tilde{f}(x) = \begin{cases} 0, & \tilde{a} \leq x < a, \\ f(x), & a \leq x \leq \tilde{b}, \\ 0, & \tilde{b} < x \leq b. \end{cases} \]

That is, we extend the domain such that traveling waves may reflect off of the Neumann boundary but not re-enter the domain of interest, \( a \leq x \leq b \), within a period \( T \) (see Appendix B for an outline of the construction). Let \( \Pi \) be the Wave-Holtz integral operator (2.4) on the original domain \( \Omega \) with impedance boundary conditions. We recall that iterates generated by \( \Pi \) at a given point, \( x \in \Omega \), are the time-average of the wave solution at \( x \) generated by the input data. Since the extended wave solution \( \tilde{w}(t, x) = w(t, x) \) for \( 0 \leq t \leq T \), we may write \( \Pi = P\Pi E \) where \( P \) is a projection operator onto the initial interval, i.e. \( P v(x) = v(x) |_{a \leq x \leq b} \), \( E \) is the extension operator such that \( [v_0, v_1]^T \to [\tilde{v}_0, \tilde{v}_1]^T \), and \( \tilde{\Pi} \) is the WaveHoltz operator on the domain \( \tilde{\Omega} \). If it can be guaranteed that \( \omega^2 \neq \lambda_j^2 \) where \( \lambda_j^2 \) is an eigenvalue of the operator \( -\partial_x(\tilde{c}^2(x) \partial_x) \), then we may prove convergence as was done for Theorem 2.4.

To show this, results on the continuity of eigenvalues of the Laplacian from [22] will be used. We present the framework of [22] needed here and consider the
following differential equation

\[
(2.16) \quad -\frac{d}{dx} \left( c^a \frac{d}{dx} y(x) \right) = \lambda y(x), \quad x \in (a', b'), \quad -\infty \leq a' < b' \leq \infty, \quad \lambda \in \mathbb{R},
\]

where \( c^a : (a', b') \to \mathbb{R} \) and \( 1/c^2 \in L^1_{\text{loc}}(a', b') \). Letting \( I = [a, b] \), \( a' < a < b < b' \) and additionally imposing the Neumann conditions \( y'(a) = y'(b) \), the above Sturm-Liouville (SL) problem is such that all eigenvalues are real, simple, and can be ordered to satisfy

\[
(2.17) \quad 0 \leq \lambda_0^2 < \lambda_1^2 < \lambda_2^2 < \ldots; \quad \lim_{n \to \infty} \lambda_n^2 = +\infty.
\]

Under the above assumptions, we state the following theorem that is proven in [22].

**Theorem 2.5** (Kong & Zettle). Let \( 1/c^2 \in L^1_{\text{loc}}(a', b') \), fix \( a', b' \), and suppose \( a, b \) are such that \( a' < a < b < b' \). Fix \( a \) and let \( \lambda_n(b) \) be an eigenvalue of the SL problem (2.16) with homogeneous Neumann boundary conditions at \( x = a \) and \( x = b \) with the corresponding eigenfunction \( u_n(x; b) \). Then the eigenvalue \( \lambda_n \in C^1([a', b']) \) satisfies the following differential equation:

\[
\frac{d}{db} \lambda_n(b) = -\lambda_n(b) u_n^2(b; b).
\]

That is, the eigenvalues of the SL problem (2.16) are differentiable functions of the endpoint \( b \). This gives us the following useful corollary.

**Corollary 2.6.** For \( n = 1, 2, \ldots \), \( \lambda_n(b) \) is a strictly decreasing function of \( b \) on \([a', b']\).

**Proof.** For homogeneous Neumann conditions, we have that \( u'_n(b; b) = 0 \). It follows that \( u_n(b; b) \neq 0 \) as otherwise \( u_n(b; b) \equiv 0 \) since \( u_n \) satisfies a linear, homogeneous second order ODE. As \( \lambda_n(b) > 0 \) for \( n > 0 \) we then have

\[
\frac{d}{db} \lambda_n(b) = -\lambda_n(b) u_n^2(b; b) < 0,
\]

so that \( \lambda_n(b) \) is a strictly decreasing function of the endpoint \( b \). \( \square \)

As a consequence of Theorem 2.5, we have

**Lemma 2.7.** Suppose \( \omega > 0 \) and that we extend \( c \) to \((a', b')\) with \( a' < a - c_n T/2 \) and \( b' > b + c_n T/2 \). Fix \( \bar{a} \in (a', a - c_n T/2) \). Then there exists an endpoint \( \bar{b} \in (b + c_n T/2, b') \) such that \( \omega^2 \neq \lambda_n(\bar{b}) \) for each \( n \in \mathbb{N}_0 \), where \( \lambda_n \) are the Neumann eigenvalues.

**Proof.** We note first that \( \bar{c} \in L^\infty(a', b') \) with \( \bar{c}(x) \geq \min(1, \gamma)c_{\min} \). Hence, \( 1/\bar{c}^2 \in L^1_{\text{loc}}(a', b') \), so Theorem 2.5 and Corollary 2.6 apply. Clearly we have \( \lambda_0(t) = 0 \) for every \( t \), and since \( \omega > 0 \) we have \( \omega^2 \neq \lambda_0(t) \). Suppose now that \( t \in (b + c_n T/2, b') \) is such that \( \omega^2 = \lambda_n(t) \) for some \( n \in \mathbb{N} \). (If not, we take \( \bar{b} = t \).) Recall that by (2.17) we have that \( \omega^2 = \lambda_n(t) < \lambda_{n+1}(t) \). Since \( \lambda_n(t), \lambda_{n+1}(t) \) are continuous, decreasing functions of the endpoint by Corollary 2.6, there necessarily exists \( \delta \in (0, b' - t) \) such that

\[
\lambda_n(t + \delta) < \omega^2 < \lambda_{n+1}(t + \delta).
\]

Letting \( \bar{b} = t + \delta \) we thus have that \( \omega^2 \neq \lambda_n(\bar{b}) \) for each \( n \in \mathbb{N}_0 \), as desired. \( \square \)
We define \( c \) in Lemma 2.3 it was shown that 
\begin{equation}
(2.19)
\end{equation}
Hence in Theorem 2.8.

By Lemma 2.7, there exists an extended wave equation (2.15) on the domain \( \Omega = [a,b] \) with homogeneous Neumann boundary conditions such that the eigenvalues \( \lambda_j \) of the Laplacian, \( -\partial_x(e^2\partial_x) \), on \( \Omega \) are not in resonance. Defining \( \hat{\lambda}_j = \lambda_j \), \( \hat{\gamma}_j = \gamma(\lambda_j) \), and \( \hat{\mu}_j = \mu(\lambda_j) \), this immediately gives that the spectral radius of the WaveHoltz operator, \( \rho = \sup_j |\hat{\mu}_j| \), is smaller than one. Moreover, the extended wave solution \( \tilde{w} \) on \( \tilde{\Omega} \) coincides with the interior impedance wave solution \( w \) on \( \Omega \) for \( t \in [0,T] \). For the extended speed function \( \hat{c} \) we have the bounds \( 0 < \hat{c}_{\min} \leq \hat{c}(x) \leq \hat{c}_{\max} < \infty \) a.e. in \( (a, b) \), where \( \hat{c}_{\min} = \min(1, \gamma)\hat{c}_{\min} \) and \( \hat{c}_{\max} = \max(1, \gamma)\hat{c}_{\max} \).

Letting \( u \) be the solution of the Helmholtz equation (2.14), we define \( q(t, x) = \cos(\omega t)[\text{Re}\{u\}, \text{Im}\{u\}]^T \) the time-harmonic Helmholtz solution in \( \Omega \) and \( \tilde{w}^n(t, x) \) the solution of (2.15) with initial data \( v_0^n, v_1^n \). Letting the error be \( e^n := [\text{Re}\{u\} - v_0^n, \omega \text{Im}\{u\} - v_1^n]^T \), it is clear the difference \( d(t, x) = q(t, x) - w(t, x) \) satisfies the unforced, homogeneous wave equation.

\[ d(t, x) = \frac{\partial}{\partial x} \left[ c^2(x) \frac{\partial d}{\partial x} \right], \quad a \leq x \leq b, \quad 0 \leq t \leq T, \]
\[ d(0, x) = e_0(x), \quad d(T, x) = e_1(x), \]
\[ \alpha d(t, a) - \beta c(x) d_x(t, a) = 0, \]
\[ \alpha d(t, b) + \beta c(x) d_x(t, b) = 0. \]

It follows that the WaveHoltz iteration applied to the error is of the form
\begin{equation}
(2.18)
\end{equation}
where \( \tilde{S} \) is defined in (2.9), but with respect to the eigenbasis of the extended Laplacian. Note that \( e_0 = [\text{Re}\{u\}, \omega \text{Im}\{u\}]^T \in H^1(\Omega) \times H^1(\Omega) \) since \( v_0^0 = v_1^0 = 0 \).

We note further that the extension operator \( E \) maps \( H^1(\Omega) \times L^2(\Omega) \) to \( H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega}) \), while for the projection operator we have \( P : H^1(\Omega) \times H^1(\Omega) \to H^1(\Omega) \times L^2(\Omega) \) and the bound
\begin{equation}
(2.19)
\end{equation}
In Lemma 2.3 it was shown that \( \tilde{S} : H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega}) \to H^1(\tilde{\Omega}) \times H^1(\tilde{\Omega}) \) and it follows that
\begin{equation}
(2.20)
\end{equation}
We define
\[ e^{n+1} = \tilde{S}Ee^n, \quad e^0 = \tilde{S}e^0, \quad e^n = \begin{bmatrix} e_0^n \\ e_1^n \end{bmatrix}. \]
Since \( e^0 \in H^1(\Omega) \times H^1(\Omega) \) it follows from (2.20) that \( \tilde{e}^n \in H^1(\tilde{\Omega}) \times H^1(\tilde{\Omega}) \) for all \( n \geq 0 \). Moreover, by rearranging the iteration (2.18) we obtain
\[
e^{n+1} = (PSE)^{n+1}e^0 = P(\tilde{S}E)^n\tilde{S}Ee^0 = P\tilde{e}^{n+1}.
\]
Then by (2.19) we have for \( n \geq 1 \),
\[
||e^n||_{H^1(\Omega) \times L^2(\Omega)} \leq ||\tilde{e}^n||_{H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega})},
\]
and to prove the stated convergence it is therefore sufficient to prove that \( \tilde{e}^n \to 0 \) in \( H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega}) \).

For the convergence we consider first the energy semi-norm \( \| \cdot \|_c \) on \( H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega}) \). Let \( \tilde{z} = [\tilde{v}_0, \tilde{v}_1]^T \in H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega}) \) and define
\[
||\tilde{z}||_c^2 := \| \tilde{\varphi} \|^2_{L^2(\tilde{\Omega})} + \| \tilde{\psi} \|^2_{L^2(\tilde{\Omega})} = \sum_{j=0}^{\infty} \tilde{\lambda}_j^2|\tilde{v}_0,j|^2 + |\tilde{v}_1,j|^2.
\]
In this semi-norm we have that
\[
||EP\tilde{z}||_c^2 = \int_{\tilde{\Omega}} \left| \tilde{\varphi} \tilde{\psi} \right|^2 dx + |EP\tilde{v}_1|^2 dx = \int_{\tilde{\Omega}} \left| \tilde{\varphi} \tilde{\psi} \right|^2 dx + |\tilde{\psi}|^2 dx 
\leq \int_{\tilde{\Omega}} \left| \tilde{\varphi} \tilde{\psi} \right|^2 dx + |\tilde{\psi}|^2 dx \leq ||\tilde{z}||_c^2.
\]

We now proceed with the proof and define \( \tilde{y} = EP\tilde{z} \), where \( \tilde{y} \) has the form
\[
\tilde{y} = EP\sum_{j=0}^{\infty} \left[ \begin{array}{cc} \tilde{v}_0,j \\ \tilde{v}_1,j \end{array} \right] \phi_j = \sum_{j=0}^{\infty} \left[ \begin{array}{cc} \tilde{y}_0,j \\ \tilde{y}_1,j \end{array} \right] \phi_j.
\]
It follows that
\[
\tilde{S}E P\tilde{z} = \sum_{j=0}^{\infty} B_j \left[ \begin{array}{cc} \tilde{y}_0,j \\ \tilde{y}_1,j \end{array} \right] \phi_j = \sum_{j=0}^{\infty} \left[ \begin{array}{cc} \tilde{y}_0,j \\ \tilde{y}_1,j \end{array} \right] \phi_j + \tilde{B}^{\text{New}} \left[ \begin{array}{cc} \tilde{y}_0,0 \\ \tilde{y}_1,0 \end{array} \right] \phi_0,
\]
so that
\[
||\tilde{S}E P\tilde{z}||_c^2 = \sum_{j=0}^{\infty} \tilde{\lambda}_j^2 \left( \tilde{\beta}_j \tilde{y}_0,j + \tilde{\gamma}_j \tilde{y}_1,j \right) \right)^2 + \sum_{j=0}^{\infty} \tilde{\lambda}_j^2 \left( \tilde{\gamma}_j \tilde{y}_0,j + \tilde{\beta}_j \tilde{y}_1,j \right) \right)^2.
\]
Since \( \tilde{\beta}_j^2 + \tilde{\gamma}_j^2 = |\tilde{\mu}_j|^2 \leq \tilde{\rho}^2 < 1 \), a simple expansion shows that
\[
||\tilde{S}E P\tilde{z}||_c^2 = \sum_{j=0}^{\infty} (\tilde{\beta}_j^2 + \tilde{\gamma}_j^2)(\tilde{\lambda}_j^2|\tilde{y}_0,j|^2 + |\tilde{y}_1,j|^2) \leq \left( \sup_j |\tilde{\mu}_j|^2 \right) \sum_{j=0}^{\infty} \tilde{\lambda}_j^2|\tilde{y}_0,j|^2 + |\tilde{y}_1,j|^2 \leq \tilde{\rho}^2 ||\tilde{y}||_c^2 \leq \tilde{\rho}^2 ||\tilde{z}||_c^2.
\]
We then obtain the estimate
\[
||\tilde{e}^n||_c^2 = ||(\tilde{S}E)^n\tilde{e}^0||_c^2 \leq \tilde{\rho}^2 ||(\tilde{S}E)^{n-1}\tilde{e}^0||_c^2 \leq \cdots \leq \tilde{\rho}^{2n} ||\tilde{e}^0||_c^2 \to 0.
\]
We now consider the full $H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega})$-norm. An application of the triangle and Poincaré inequality (with constant $C_p$) gives

\begin{equation}
\|\tilde{e}^n\|_{H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega})}^2 = \|\partial_x \tilde{e}^n_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^n_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^n_1\|_{L^2(\tilde{\Omega})}^2 \\
\leq \|\partial_x \tilde{e}^n_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^n_0 - \tilde{e}^{0,0}_0\phi_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^{0,0}_0\phi_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^n_1\|_{L^2(\tilde{\Omega})}^2 \\
\leq (1 + C_P)\|\partial_x \tilde{e}^n_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^n_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{e}^n_1\|_{L^2(\tilde{\Omega})}^2,
\end{equation}

where $\phi_0$ is a constant eigenfunction of the Laplacian (and thus of $\tilde{S}$) with eigenvalue $\lambda_0 = 0$. To obtain convergence in $H^1(\Omega) \times L^2(\Omega)$ of the error $\tilde{e}^n$ we must thus examine the convergence of $\tilde{e}^{0,0}_0$ separately.

Before proceeding, we require the following lemma:

**Lemma 2.9.** Let $\tilde{z} \in H^1(\tilde{\Omega}) \times L^2(\tilde{\Omega})$. Then

$$\|EPz - \tilde{z}\|_{L^2(\tilde{\Omega}) \times L^2(\tilde{\Omega})} \leq C_1 \|\tilde{z}\|_2,$$

where $C_1 = \max\{2(a - \tilde{a})/\tilde{e}^{\min}_2, 2(\tilde{b} - b)/\tilde{e}^{\min}_2, 1\} > 0$.

**Proof.** Let $\tilde{z} = [\tilde{v}_0, \tilde{v}_1]^T$ with $\tilde{v}_0 \in H^1(\tilde{\Omega})$ and $\tilde{v}_1 \in L^2(\tilde{\Omega})$. Then

$$\|EPz - \tilde{z}\|_{L^2(\tilde{\Omega}) \times L^2(\tilde{\Omega})}^2 = \int_a^b \int_a^b |\tilde{v}_0(x) - \tilde{v}_0(a)|^2 + |\tilde{v}_1(x)|^2 \, dx \, ds \\
+ \int_b^\tilde{b} \int_a^b |\tilde{v}_0(x) - \tilde{v}_0(b)|^2 + |\tilde{v}_1(x)|^2 \, dx \, ds \\
\leq \int_a^\tilde{a} \int_a^x |\partial_x \tilde{v}_0(s)|^2 \, ds \, dx + \int_b^\tilde{b} \int_b^x |\partial_x \tilde{v}_0(s)|^2 \, ds \, dx + \int_a^\tilde{a} \int_a^x |\partial_x \tilde{v}_0(s)|^2 \, ds \, dx \\
+ \|\tilde{v}_1\|_{L^2(\tilde{\Omega})}^2,$$

since $\tilde{v}_0 \in H^1(\tilde{\Omega})$. Moreover,

$$\int_a^\tilde{a} \int_a^x |\partial_x \tilde{v}_0(s)|^2 \, ds \, dx \leq \int_a^\tilde{a} \int_a^x (|\partial_x \tilde{v}_0(s)|^2 + |\partial_x \tilde{v}_0(s)|^2) \, ds \, dx \leq \int_a^\tilde{a} \frac{1}{\tilde{e}^{\min}_2} \|\tilde{v}_0\|_{L^2(\tilde{\Omega})}^2 \, dx \\
\leq \frac{a - \tilde{a}}{\tilde{e}^{\min}_2} \|\partial_x \tilde{v}_0\|_{L^2(\tilde{\Omega})}^2.$$

A similar estimate for the integral in the left part of the extended domain, $x \in [b, \tilde{b}]$, gives the bound

$$\|EPz - \tilde{z}\|_{L^2(\tilde{\Omega}) \times L^2(\tilde{\Omega})}^2 \leq C_1 \|\tilde{v}_0\|_{L^2(\tilde{\Omega})}^2 + \|\tilde{v}_1\|_{L^2(\tilde{\Omega})}^2 \leq C_1 \|\tilde{z}\|_2^2,$$

as desired. \hfill \square

To simplify notation we define

$$I_0 \begin{bmatrix} \tilde{v}_0 \\ \tilde{v}_1 \end{bmatrix} := \tilde{v}_0, \quad I_0^* \tilde{v}_0 := \begin{bmatrix} \tilde{v}_0 \\ 0 \end{bmatrix}, \quad \langle f, g \rangle := \int_a^\tilde{b} f(x) g(x) \, dx,$$
so that we may write the constant component of the $\varepsilon^0$ error as

$$
\varepsilon^{n+1}_{0,0} = \langle I_0 \varepsilon_0^{n+1}, \phi_0 \rangle = \langle I_0 \tilde{S}EP\varepsilon^n, \phi_0 \rangle = \langle I_0 \tilde{S}(EP\varepsilon^n - \varepsilon^n), \phi_0 \rangle + \langle I_0 \tilde{S}(I - I_0^* I_0)\varepsilon^n, \phi_0 \rangle + \langle I_0 \tilde{S}I_0^* I_0 \varepsilon^n, \phi_0 \rangle.
$$

For the last term we get, since $B_0 = B_0^{\text{Neu}}$,

$$
\langle I_0 \tilde{S}I_0^* I_0 \varepsilon^n, \phi_0 \rangle = \left(\sum_{j=0}^{\infty} B_j I_0^* I_0 \left[ \frac{\varepsilon^n_{0,j}}{\varepsilon_{1,0}} \right] \phi_j, \phi_0 \right) = I_0 B_0^{\text{Neu}} I_0^* I_0 \left[ \frac{\varepsilon^n_{0,0}}{\varepsilon_{1,0}} \right] = -\frac{1}{2} \varepsilon^{n}_{0,0}.
$$

Furthermore, we have

$$
\|I_0 \tilde{S} \tilde{z}\|_{L^2(\tilde{\Omega})} \leq \|\tilde{S} \tilde{z}\|_{L^2(\tilde{\Omega})} \leq \|\tilde{S} \tilde{z}\|_{L^2(\tilde{\Omega})} \leq C_2 \|\tilde{z}\|_{L^2(\tilde{\Omega})} \times L^2(\tilde{\Omega}),
$$

for some constant $C_2$, since $\tilde{S}$ is a bounded linear map from $L^2(\tilde{\Omega}) \times L^2(\tilde{\Omega})$ to $L^2(\tilde{\Omega}) \times L^2(\tilde{\Omega})$ by Lemma 2.3. Then applications of the Cauchy-Schwarz, triangle inequality and Lemma 2.9 give

$$
|\varepsilon^{n+1}_{0,0}| \leq \|I_0 \tilde{S}(EP\varepsilon^n - \varepsilon^n, \phi_0)\| + \|I_0 \tilde{S}(I - I_0^* I_0)\varepsilon^n, \phi_0\| + \|I_0 \tilde{S}I_0^* I_0 \varepsilon^n, \phi_0\|
$$

$$
\leq C_2 \|EP\varepsilon^n - \varepsilon^n\|_{L^2(\tilde{\Omega})} \times L^2(\tilde{\Omega}) + C_2 \|(I - I_0^* I_0)\varepsilon^n\|_{L^2(\tilde{\Omega})} \times L^2(\tilde{\Omega}) + \frac{1}{2} \varepsilon^n_{0,0}
$$

$$
\leq A \|\varepsilon^n\| + \frac{1}{2} \varepsilon^n_{0,0} \leq A \tilde{\rho}^{n+1} + \frac{1}{2} \varepsilon^n_{0,0},
$$

where $A = C_2 \sqrt{C_1} > 0$ and $C_1 = \max\{(a - \tilde{a})/\tilde{\varepsilon}_{\text{min}}^2, (b - \tilde{b})/\tilde{\varepsilon}_{\text{min}}^2, 1\} > 0$.

Without loss of generality we assume $\tilde{\rho} \neq 1/2$ since it is possible to choose $\tilde{a}, \tilde{b}$ such that the problem is not at resonance with $\tilde{\rho} \neq 1/2$. We define the sequence

$$
y_n = \frac{\varepsilon^n_{0,0}}{A} - \frac{\tilde{\rho}^{n}}{\tilde{\rho} - 1/2}.
$$

Then

$$
y_{n+1} = \frac{\varepsilon^{n+1}_{0,0}}{A} - \frac{\tilde{\rho}^{n+1}}{\tilde{\rho} - 1/2} \leq A \tilde{\rho}^{n+1} + \frac{1}{2} \varepsilon^n_{0,0} - \frac{\tilde{\rho}^{n+1}}{\tilde{\rho} - 1/2}
$$

$$
= \frac{1}{2} \left( \frac{\varepsilon^n_{0,0}}{A} - \frac{\tilde{\rho}^{n}}{\tilde{\rho} - 1/2} \right) = \frac{1}{2} y_n.
$$

Therefore $y_n \leq 2^{-n} y_0$ so that

$$
\lim_{n \to \infty} \varepsilon^n_{0,0} = \lim_{n \to \infty} A \left( y_n + \frac{\tilde{\rho}^{n}}{\tilde{\rho} - 1/2} \right) = 0.
$$

Taking a limit of (2.21) gives that $\|\varepsilon^n\|_{H^1(\tilde{\Omega})} \to 0$, so that we obtain convergence of the iteration in $H^1(\Omega) \times L^2(\Omega)$. \hfill \Box

**Remark 2.10.** The above analysis is for a single spatial dimension, but we note that it in certain situations it may be extended to higher dimensions. For instance, interior impedance problems with constant coefficients and simple geometries may be extended by an appropriate enclosing box from which the above arguments can give convergence. In general, it is difficult to prove convergence in higher dimensions in this way as care needs to be taken to make appropriate wavespeed extensions that avoid reflections due to potentially discontinuous wavespeeds close to boundaries with impedance conditions.
3. Damped Wave/Helmholtz Equation

As mentioned in the introduction, a popular preconditioning approach for solving Helmholtz problems is to introduce a damping term as in the shifted Laplacian preconditioners [11]. In this section we similarly consider the complex-valued damped wave equation

\[ w_{tt} + \eta w_t = \nabla \cdot [c^2(x) \nabla w] - f(x)e^{-i\omega t}, \quad \eta > 0, \]

for which we note that if \( w(t, x) = u(x) e^{-i\omega t} \) then

\[ \nabla \cdot [c^2(x) \nabla u] + (\omega^2 + i\eta \omega) u = f(x), \]

so that we essentially have added a purely imaginary shift of the Laplacian

\[ L = -\nabla \cdot [c^2(x) \nabla] - i\eta \omega. \]

Here we consider only problems with energy conserving boundary conditions (i.e. Dirichlet or Neumann), and as a result of the imaginary shift of the Laplacian we note there are no longer resonant frequencies. While for the sake of simplicity we consider the complex-valued problem in this section, in practice we solve the real-valued problem as presented in Section 2 with the filter (2.4). For the above complex-valued problem, we may then similarly prove an analogous result to Theorem 2.4.

Theorem 3.1. The iteration (2.6) with the complex-valued filter

\[
(3.1) \quad \Pi \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \frac{1}{T} \int_0^T e^{i\omega t} \begin{bmatrix} w(t, x) \\ w_t(t, x) \end{bmatrix} dt, \quad T = \frac{2\pi}{\omega},
\]

converges for every \( \eta > 0 \) with a convergence rate bounded by \( 2(1 - e^{-\eta T/2})/\eta T \).

Proof. Suppose \((\lambda^2_j, \phi_j)\) are the eigenmodes of the real-valued Laplacian in the domain \( \Omega \). We note that the shifted Laplacian now has a spectrum that is \( \lambda^2_j - i\eta \omega \). Expanding in terms of this basis and taking inner products, we can see that

\[ (\omega^2 + i\eta \omega - \lambda^2_j)u_j = f_j, \]

where we expand the real and imaginary parts of \( u \) and \( f \) as \( u_j = u_j^R + iu_j^I \) and \( f_j = f_j^R + if_j^I \). Let the damped wave equation solution have the form

\[ \sum_{n=0}^{\infty} w_j(t) \phi_j(x). \]

Defining \( \alpha_j = \sqrt{4\lambda^2_j - \eta^2/2} \), then the solution can be shown to be given by

\[
w_j(t) = u_j \left( e^{-i\omega t} - e^{-\eta t} \left[ \cos(\alpha_j t) + \frac{\eta - 2i\omega}{2\alpha_j} \sin(\alpha_j t) \right] \right) + e^{-\eta t} \left( v_0,j \cos(\alpha_j t) + \frac{\eta \sin(\alpha_j t)}{2\alpha_j} + \frac{v_1,j \sin(\alpha_j t)}{\alpha_j} \right),
\]

from which we note that we arrive at exactly the same set of coefficients as in the previous analysis if \( \eta = 0 \) and the real part of the solution is taken. Using the complex-valued filters

\[
\hat{\beta}(\alpha) := \frac{1}{T} \int_0^T e^{(i\omega - \eta/2)t} \cos(\alpha t) dt, \quad \hat{\gamma}(\alpha) := \frac{1}{T} \int_0^T e^{(i\omega - \eta/2)t} \sin(\alpha t) dt,
\]

we have

\[
\Pi \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \begin{bmatrix} \hat{\beta}(\alpha) \\ \hat{\gamma}(\alpha) \end{bmatrix} \begin{bmatrix} \beta_0 \\ \gamma_0 \end{bmatrix}, \quad \beta_0 := \frac{1}{T} \int_0^T e^{-(i\omega - \eta/2)t} \cos(\alpha t) dt, \quad \gamma_0 := \frac{1}{T} \int_0^T e^{-(i\omega - \eta/2)t} \sin(\alpha t) dt.
\]
we can write the iteration as
\begin{equation}
(3.2) \quad \begin{pmatrix} v_{0,j}^{n+1} \\ v_{1,j}^{n+1} \end{pmatrix} = \Pi \begin{pmatrix} v_{0,j}^{n} \\ v_{1,j}^{n} \end{pmatrix} = \left( I - \hat{B}_j \right) \begin{pmatrix} u_j \\ i\omega u_j \end{pmatrix} + \hat{B}_j \begin{pmatrix} v_{0,j}^{n} \\ v_{1,j}^{n} \end{pmatrix},
\end{equation}
where if \( \hat{\beta}_j = \hat{\beta}(\alpha_j) \) and \( \hat{\gamma}_j = \hat{\gamma}(\alpha_j) \) then
\[ \hat{B}_j = \begin{pmatrix} \hat{\beta}_j + \frac{\eta}{2\alpha_j^2} \hat{\gamma}_j & \hat{\gamma}_j/\alpha_j \\ -(\alpha_j + \frac{\eta}{2\alpha_j}) \hat{\gamma}_j & \hat{\beta}_j - \frac{\eta}{2\alpha_j} \hat{\gamma}_j \end{pmatrix}. \]
As in the previous analysis, we require that the spectral radius of \( \hat{B}_j \) be less than one. The eigenvalues are given by \( \hat{\mu}_j = \hat{\beta}_j \pm i\hat{\gamma}_j \) so that by definition
\begin{equation}
(3.3) \quad |\hat{\mu}_j| = |\hat{\beta}_j \pm i\hat{\gamma}_j| = \left| \frac{1}{T} \int_0^T e^{\omega(+\alpha_j)t} e^{-\eta t/2} \, dt \right| \leq \frac{2}{\eta T} (1 - e^{-\eta T/2}) < 1,
\end{equation}
given that \( \eta > 0 \).

Thus the iteration always converges in the damped case without extra conditions on the eigenvalues. From (3.3) we see that for a desired fixed rate of convergence the damping parameter \( \eta \) must grow proportionally to \( \omega \) since \( \eta T \sim \eta/\omega \), and that frequency-independent convergence is achieved by choosing \( \eta = O(\omega) \).

**Remark 3.2.** We note that in this section we use the complex-valued filter \( e^{i\omega t}/T \) instead of the usual filter, \( 2(\cos(\omega t) - 1/4)/T \). The choice of filter in (3.1), as well as performing the analysis using complex arithmetic, was done for the sake of simplicity. The choice of filter need not be restricted to \( 2(\cos(\omega t) - 1/4)/T \), we refer the reader to Section 2.3 and 4.1.4 of [5] for further discussion on the choice of filter.

4. **Analysis of Higher Order Time-Stepping Schemes for the Discrete Iteration**

We introduce the temporal grid points \( t_n = n\Delta t \) and a spatial grid with \( N \) points together with the vector \( w^n \in \mathbb{R}^N \) containing the grid function values of the approximation at \( t = t_n \). We also let \( f \in \mathbb{R}^N \) hold the corresponding values of the right hand side. The discretization of the continuous spatial operator \( -\nabla \cdot (c^2(x) \nabla) \), including the boundary conditions, is denoted \( L_h \) and it can be represented as an \( N \times N \) matrix. The values \( -\nabla \cdot (c^2(x) \nabla u) \) are then approximated by \( L_h w^n \). 

As in the continuous case, we assume \( L_h \) has the eigenmodes \( (\lambda_j^2, \phi_j) \), such that \( L_h \phi_j = \lambda_j^2 \phi_j \) for \( j = 1, \ldots, N \), where all \( \lambda_j \) are real, strictly positive and ordered as \( 0 \leq \lambda_1 \leq \ldots \leq \lambda_N \).

We let the discrete Helmholtz solution \( u \) be defined through
\[-L_h u + \omega^2 u = f.\]

The numerical approximation of the iteration operator is denoted \( \Pi_h \), and it is implemented as follows. Given \( v \in \mathbb{R}^N \), we use the leap frog method to solve the wave equation and add in higher order corrections as in the Modified Equation (ME) approach [30, 2]. For a general \( 2m \) scheme, recall that via Taylor expansion
\[ \frac{w^{n+1} - 2w^n + w^{n-1}}{\Delta t^2} = w_{tt} + 2 \sum_{k=2}^{\infty} \frac{\Delta t^{2(k-1)}}{(2k)!} \frac{\partial^{2k}}{\partial t^{2k}} w^n. \]
Then using the PDE to convert time derivatives to spatial derivatives we get the expression
\[
\frac{\partial^{2k}}{\partial t^{2k}} w^n \approx L_h^k w^n + \cos(\omega t_n) \sum_{\ell=0}^{k-1} (-1)^{k+\ell} \omega^{2(k-\ell-1)} L_h^\ell f,
\]
for \( k = 1, 2, \ldots \). Then for a 2m order scheme we have
\[
\frac{w^{n+1} - 2w^n + w^{n-1}}{\Delta t^2} - 2 \sum_{k=2}^{m} \frac{\Delta t^{2k-2}}{(2k)!} \left[ L_h^k w^n + \cos(\omega t_n) \sum_{\ell=0}^{k-1} (-1)^{k+\ell} \omega^{2(k-\ell-1)} L_h^\ell f \right] = L_h w^n - f \cos(\omega t_n),
\]
with time-step \( \Delta t = T/M \) for some integer \( M \), and initial data
\[
w^0 = v, \quad w^{-1} = v + \sum_{k=1}^{m} \frac{(-1)^k \Delta t^{2k}}{(2k)!} \left[ -L_h^k v + \sum_{\ell=0}^{k-1} (-1)^{\ell+1} \omega^{2(k-\ell-1)} L_h^\ell f \right].
\]
The trapezoidal rule is then used to compute \( \Pi_h v \),
\[
\Pi_h v = \frac{2\Delta t}{T} \sum_{n=0}^{M} \eta_n \left( \cos(\omega t_n) - \frac{1}{4} \right) w^n, \quad \eta_n = \begin{cases} \frac{1}{2}, & n = 0 \text{ or } n = M, \\ 1, & 0 < n < M. \end{cases}
\]
We may then prove the following theorem that is a generalization of Theorem 2.4 of [5].

**Theorem 4.1.** Suppose that \( L_h \) has real and strictly positive eigenvalues \( \lambda_j \) and that there are no resonances, such that \( \delta_h = \min_j |\lambda_j - \omega|/\omega > 0 \). Moreover, assume that \( \Delta t \) satisfies the stability and accuracy requirements
\[
\Delta t < \frac{2}{\lambda_N + 2\omega/\pi}, \quad \Delta t \omega \leq \min(\delta_h, 1).
\]
Then the fixed point iteration \( v^{(k+1)} = \Pi_h v^{(k)} \) with \( v^{(0)} = 0 \) converges to \( v^\infty \) which is a solution to the discretized Helmholtz equation,
\[-L_h v^\infty + \tilde{\omega}^2 v^\infty = f,
\]
with the modified frequency \( \tilde{\omega} \), defined as the smallest positive real number satisfying
\[
\sin^2(\omega \Delta t/2) = \sum_{j=1}^{m} \frac{(-1)^{j+1} (\Delta t \tilde{\omega})^{2j}}{(2j)!},
\]
where 2m is the order of the ME time-stepping scheme. Moreover, there are constants \( C_m < 1 \) and \( C'_m \) only depending on m such that
\[
|\omega - \tilde{\omega}| \leq C_m \Delta t^{2m \omega^{2m+1}} , \quad \|u - v^\infty\|_2 \leq C'_m \Delta t^{2m \omega^{2m-2}} \|f\|_2.
\]
The convergence rate is at least \( \rho_h = \max(1 - 0.3\delta_h^2, 0.6) \).

**Proof.** We expand all functions in eigenmodes of \( L_h \),
\[
w^n = \sum_{j=1}^{N} w^n_j \phi_j, \quad f = \sum_{j=1}^{N} f_j \phi_j, \quad u = \sum_{j=1}^{N} u_j \phi_j, \quad v = \sum_{j=1}^{N} v_j \phi_j, \quad v^\infty = \sum_{j=1}^{N} v^\infty_j \phi_j.
\]
Then the Helmholtz eigenmodes of $u$ and $v^\infty$ satisfy

$$u_j = \frac{f_j}{\omega^2 - \lambda_j^2}, \quad v_j^\infty = \frac{f_j}{\omega^2 - \lambda_j^2}.$$

We note that $\tilde{\omega}$ is well-defined by Lemma C.1 in Appendix C. The same lemma also shows the bound on $|\omega - \tilde{\omega}|$, which implies that $\tilde{\omega}$ is not resonant and $v_j^\infty$ is well-defined for all $j$, since by (C.8) and (4.3)

$$|\tilde{\omega} - \lambda_j| \geq |\omega - \lambda_j| - |\omega - \tilde{\omega}| \geq \omega \delta_h - C_m \Delta t^{2m} \omega^{2m+1} \geq \omega \left(\delta_h - C_m \min(\delta_h, 1)^{2m}\right) \geq \omega \delta_h (1 - C_m) > 0.$$

The wave solution eigenmodes to (4.1) are given by the difference equation

$$(4.4) \quad w_j^{n+1} - 2w_j^n + w_j^{n-1} + 2 \left[ \sum_{k=1}^{m} \frac{(-1)^{k+1} \Delta t^{2k} \lambda_j^{2k}}{(2k)!} \right] w_j^n = 2 \left[ \sum_{k=1}^{m} \frac{(-1)^k \Delta t^{2k}}{(2k)!} \sum_{\ell=0}^{k-1} \omega^{2(k-\ell-1)} \lambda_j^{2\ell} \right] f_j \cos(\omega t_n),$$

with initial data

$$w_j^0 = v_j, \quad w_j^{-1} = v_j \left(1 + \sum_{k=1}^{m} \frac{(-1)^k \Delta t^{2k}}{(2k)!} \lambda_j^{2k}\right) + f_j \left[ \sum_{k=1}^{m} \frac{(-1)^k \Delta t^{2k}}{(2k)!} \sum_{\ell=0}^{k-1} \omega^{2(k-\ell-1)} \lambda_j^{2\ell}\right].$$

By (4.3), the discrete solution is stable and given by

$$(4.5) \quad w_j^n = (v_j - v_j^\infty) \cos(\tilde{\lambda}_j t_n) + v_j^\infty \cos(\omega t_n),$$

where $\tilde{\lambda}_j$ is well-defined, by (C.3), as the smallest positive real number satisfying

$$(4.6) \quad \sin^2(\tilde{\lambda}_j \Delta t/2) \geq \sum_{k=1}^{m} \frac{(-1)^{k+1} (\Delta t \tilde{\lambda}_j)^{2k}}{2(2k)!}.$$

For $m \geq 2$, we have that $|\omega - \tilde{\omega}| \leq C_m \Delta t^{2m} \omega^{2m+1} \leq \Delta t^2 \omega^3/24$ since $C_m = 5/(2m + 2)! \leq 1/24$ by Lemma C.1. We may then apply the following lemma, restated from [5], to obtain convergence of the discrete iteration (we note that the proof of Lemma 4.2 requires a simple modification for the case $m = 1$ and is thus not presented here for the sake of brevity).

**Lemma 4.2.** Under the assumptions of Theorem 4.1,

$$(4.7) \quad \max_{1 \leq j \leq N} |\beta_h(\tilde{\lambda}_j)| \leq \rho_h =: \max(1 - 0.3\delta_h^2, 0.6).$$
Letting \( e = u - v^\infty \) be the error in the discrete solutions, the components of the error in the basis of the Laplacian satisfy

\[
|e_j| = |u_j - v^\infty_j| = \left| f_j \left( \frac{1}{\omega^2 - \lambda_j^2} - \frac{1}{\tilde{\omega}^2 - \lambda_j^2} \right) \right|
\]

\[
= |f_j (\tilde{\omega} - \omega)\left| \frac{\omega + \lambda_j}{(\omega + \lambda_j)(\omega - \lambda_j)(\tilde{\omega} - \lambda_j)} \right|
\]

\[
\leq C_m |f_j| |\Delta t^{2m} \omega^{2m+1}| \left| \frac{\omega^{-1} + \tilde{\omega}^{-1}}{(1 - C_m)\delta_h^2} \right|
\]

\[
\leq C_m (2 - C_m)^{-1} |f_j| |\Delta t^{2m} \omega^{2m} \delta_h^{-2}| =: C'_m |f_j| |\Delta t^{2m} \omega^{2m} \delta_h^{-2}|
\]

where we also used the fact that

\[
\frac{\omega}{\tilde{\omega}} = \frac{\omega}{\omega + \tilde{\omega} - \omega} \leq \frac{\omega}{1 - C_m \Delta t^{2m} \omega^{2m+1}} = \frac{1}{1 - C_m \Delta t^{2m} \omega^{2m}} \leq \frac{1}{1 - C_m}
\]

This gives

\[
\|u - v^\infty\|_2 = \|e\|_2 \leq C'_m \|\Delta t^{2m} \omega^{2m} \delta_h^{-2}\|f\|_2
\]

concluding the proof of the theorem.

**Remark 4.3.** As alluded to in Remark 6 of [5], knowledge of how a particular discretization approximates the eigenvalues of the continuous operator can be used to improve the iteration. In fact, the above error due to time discretization can be removed by defining \( \tilde{\omega} \) by the relation

\[
\sin^2(\frac{\omega \Delta t}{2}) = \sum_{k=1}^{m} \frac{(-1)^{k+1} (\Delta t \omega)^{2k}}{2(2k)!}.
\]

Then using \( f \cos(\tilde{\omega} t_n) \) instead of \( f \cos(\omega t_n) \) in the time-stepping (4.1), in addition to the modified trapezoidal quadrature rule (first introduced in [28])

\[
(4.8)
\]

\[
\Pi_h v = \frac{2\Delta t}{T} \sum_{n=0}^{M} \eta_n \frac{\cos(\omega t_n)}{\cos(\tilde{\omega} t_n)} \left( \cos(\omega t_n) - \frac{1}{4} \right) w^n, \quad \eta_n = \begin{cases} \frac{1}{2}, & n = 0 \text{ or } n = M, \\ 1, & 0 < n < M, \end{cases}
\]

gives that the limit will be precisely the discrete Helmholtz solution, \( v^\infty = u \), as long as the time-step size is chosen so that \( \cos(\tilde{\omega} t_n) \neq 0 \). Moreover, the first time-step restriction of (4.3) arising from the usual CFL condition for the second order scheme may be relaxed (expressions for which may be found in [16]) though the condition \( \Delta t \omega \leq \min(\delta_h, 1) \) may be more restrictive for problems close to resonance. We additionally note that in [32] an alternative approach to remove time-discretization error was presented, however the approach modified the time-stepping scheme whereas we modify the frequency of the forcing and update our quadrature rule.

5. Wave Equation Solvers

In this section we briefly outline the numerical methods we use in the experimental section below. We consider both discontinuous Galerkin finite element solvers and finite difference solvers. In all the experiments we always use the trapezoidal rule to compute the integral in the WaveHoltz iteration.
5.1. The Energy Based Discontinuous Galerkin Method. Our spatial discretization is a direct application of the formulation described for general second order wave equations in [3, 4]. Here we outline the spatial discretization for the special case of the scalar wave equation in one dimension and refer the reader to [3] for the general case.

The energy of the scalar wave equation is

\[ H(t) = \int_D v^2 + G(x, w_x) dx, \]

where

\[ G(x, w_x) = \frac{c^2(x) w_x^2}{2}, \]

is the potential energy density, \( v \) is the velocity (not to be confused with the iterates \( v^n \) above) or the time derivative of the displacement, \( v = w_t \). The wave equation, written as a second order equation in space and first order in time then takes the form

\[ w_t = v, \]
\[ v_t = -\delta G, \]

where \( \delta G \) is the variational derivative of the potential energy

\[ \delta G = -(G_{w_x})_x = -(c^2(x) w_x)_x. \]

For the continuous problem the change in energy is

\[ \frac{dH(t)}{dt} = \int_D v w_t + \frac{1}{2} \frac{\partial}{\partial t} \left( c^2 w_x \right) dx = [w_t(c^2 w_x)]_{\partial D}, \]

where the last equality follows from integration by parts together with the wave equation. Now, a variational formulation that mimics the above energy identity can be obtained if the equation \( v - w_t = 0 \) is tested with the variational derivative of the potential energy. Let \( \Omega_j \) be an element and \( \Pi^s(\Omega_j) \) be the space of polynomials of degree \( s \), then the variational formulation on that element is:

**Problem 1.** Find \( v^h \in \Pi^s(\Omega_j), w^h \in \Pi^r(\Omega_j) \) such that for all \( \psi \in \Pi^s(\Omega_j), \phi \in \Pi^r(\Omega_j) \)

\[ \int_{\Omega_j} c^2 \phi_x \left( \frac{\partial w^h}{\partial t} - v^h \right) dx = [\phi(c^2 w_x)]_{\partial \Omega_j}, \]
\[ \int_{\Omega_j} \psi \frac{\partial w^h}{\partial t} + c^2 \psi_x \cdot w^h dx = [\psi(c^2 w_x)]_{\partial \Omega_j}. \]

Let \([f]\) and \( \{f\} \) denote the jump and average of a quantity \( f \) at the interface between two elements, then, choosing the numerical fluxes as

\[ v^* = \{v\} - \tau_1[(c^2 w_x)] \]
\[ (c^2 w_x)^* = \{c^2 w_x\} - \tau_2[[v]], \]

will yields a contribution \(-\tau_1((c^2 w_x))^2 - \tau_2([[v]])^2\) from each element face to the change of the discrete energy

\[ \frac{dH^h(t)}{dt} = \frac{d}{dt} \sum_j \int_{\Omega_j} \frac{(v^h)^2}{2} + G(x, w^h_x). \]
Physical boundary conditions can also be handled by appropriate specification of the numerical fluxes, see [3] for details. The above variational formulation and choice of numerical fluxes results in an energy identity similar to (5.1). However, as the energy is invariant to certain transformations the variational problem does not fully determine the time derivatives of \( w^h \) on each element and independent equations must be introduced. In this case there is one invariant and an independent equation is \( \int_{\Omega} \left( \frac{\partial w^h}{\partial t} - v^h \right) \, dx = 0 \). For the general case and for the elastic wave equation see [3] and [4].

In this paper we always choose \( \tau_i > 0 \) (so-called upwind or Sommerfeld fluxes) and we always choose the approximation spaces to be of the same degree \( r = s \). These choices result in methods that are \( r + 1 \) order accurate in space.

5.2. Symmetric Interior Penalty Discontinuous Galerkin Method. In addition to the above energy DG method, we also consider the Symmetric Interior Penalty DG (SIPDG) discretization, [18], for examples in two dimensions. The bilinear form in this case is

\[
a_h(u, v) = \sum_{K \in T_h} \int_K c^2 \nabla u \cdot \nabla v \, dx - \sum_{f \in F_h} \int_f \llbracket u \rrbracket \cdot \{ c^2 \nabla v \} - \llbracket v \rrbracket \cdot \{ c^2 \nabla u \} + \gamma h_F^{-1} c^2 \llbracket u \rrbracket \cdot \llbracket v \rrbracket \, ds,
\]

where \( T_h \) is a collection of triangular elements, \( F_h \) is the collection of element faces, \( h_F \) is the diameter of the edge or face \( F \), and \( \gamma \) is the interior penalty stabilization parameter which must be chosen to be sufficiently large to ensure the system is positive-definite.

5.3. Finite Difference Discretizations. For the finite difference examples in a single dimension, we consider discretizations by uniform grids \( x_i = x_L + i h_x \), with \( i = -1, \ldots, n+1 \) and \( h_x = (x_R - x_L)/n \). To impose impedance boundary conditions of the form \( w \pm \vec{n} \cdot \nabla w = 0 \) we evolve the wave equation as a first order system in time according to the semi-discrete approximation

\[
\frac{d}{dt} w_i(t) = (D_+ D_-) w_i, \quad \frac{d}{dt} v_i(t) = v_i,
\]

and for the boundaries we find the ghost point values by enforcing

\[
(5.4) \quad v_0 - D_0 w_0 = 0, \quad v_n - D_0 w_n = 0.
\]

Here we have used the standard forward, backward and centered finite difference operators, for example \( h D_+ w_i = w_{i+1} - w_i \) etc.

5.4. Time Discretization. For some of the numerical examples in a single dimension, we use either an explicit second order accurate centered discretization of \( w_{tt} \) or use the higher order corrected ME methods described in Section 4.

For the DG discretizations we employ Taylor series time-stepping in order to match the order of accuracy in space and time. Assuming that all the degrees of freedom have been assembled into a vector \( w \) we can write the semi-discrete method as \( w_t = Q w \) with \( Q \) being a matrix representing the spatial discretization. Assuming we know the discrete solution at the time \( t_n \) we can advance it to the
next time-step $t_{n+1} = t_n + \Delta t$ by the simple formula
\[
w(t_n + \Delta t) = w(t_n) + \Delta t w_t(t_n) + \frac{(\Delta t)^2}{2!} w_{tt}(t_n) \ldots
\]
\[
= w(t_n) + \Delta t Q w(t_n) + \frac{(\Delta t)^2}{2!} Q^2 w(t_n) \ldots.
\]
The stability domain of the Taylor series which truncates at time derivative number $N_T$ includes the imaginary axis if $\text{mod}(N_T, 4) = 3$ or $\text{mod}(N_T, 4) = 0$. However as we use a slightly dissipative spatial discretization the spectrum of our discrete operator will be contained in the stability domain of all sufficiently large choices of $N_T$ (i.e. the $N_T$ should not be smaller than the spatial order of approximation).

6. Numerical Examples

In this section we illustrate the properties of the proposed iteration and its Krylov accelerated version by a sequence of numerical experiments in one and two spatial dimensions.

6.1. Examples in One Dimension.

6.1.1. Convergence Rate for Impedance Boundary Conditions. In [5], an application of Weyl asymptotics [34] revealed that the minimal relative gap to resonance, $\delta = \min_j |\omega - \lambda_j|/\omega$ where $\lambda_j^2$ are the eigenvalues of the Laplacian, shrinks as $\omega^{-d}$ where $d$ is the spatial dimension of the Helmholtz problem of interest. Analysis of the symmetric, positive definite formulation of the iteration then yielded a convergence rate of $1 - O(\delta^2) \approx 1 - O(\omega^{-2d})$. However, numerical experiments with Helmholtz problems with certain open/outflow boundary conditions suggest a much more attractive convergence rate than the unacceptable $1 - O(\omega^{-2d})$ rate. A natural question then is whether or not this seemingly pessimistic convergence rate can be observed for outflow boundary conditions which are much more common in practical applications.

To that end, we consider a set of sample Helmholtz problems in a single spatial dimension with a constant (normalized) speed of sound, $c = 1$, in the domain $0 \leq x \leq 2$ where we impose the impedance boundary condition $w_t + \vec{n} \cdot w_x = 0$, which we note is equivalent to the Sommerfeld radiation condition. The Helmholtz problem under consideration has no forcing and so $f = 0$. We formulate the wave equation in first order form and apply the extended iteration (2.6) since the boundary conditions do not conserve energy. The Laplacian is discretized with a standard three-point finite difference approximation, and a fourth order Taylor scheme is used for time-stepping. We define the initial conditions as
\[
v_0(x) = \sin(\omega x) - \frac{1}{2} (\sin((\omega + 2\pi)x) + \sin((\omega - 2\pi)x)), \quad v_1(x) = -\frac{d}{dx} v_0(x),
\]
which are shown in Figure 1.

By definition, $\|S\|_2 = \sup\|z\|_2 \neq 0 \|Sz\|_2/\|z\|_2 \geq \|Sz^0\|_2/\|z^0\|_2$ so that if $\|Sz^0\|_2/\|z^0\| \approx 1 - O(\omega^{-2})$ is observed then the estimate of the spectral radius of the fixed point operator $S$ is tight even for the problem with impedance boundary conditions. We consider a sweep of Helmholtz frequencies $\omega = 10\pi, 15\pi, 20\pi, \ldots, 120\pi$ with fifty points per wavelength and a CFL number of $10^{-1}$ for the solution of the wave equation. The results of this experiment are shown in Figure 1.
On the left of Figure 1 we see the first part of the initial condition \(v^0\) for a frequency of \(\omega = 10\pi\). We note that this specific initial condition is constructed such that it is close to a resonant mode – which the filter-transfer function \(\beta\) weakly damps – as well as being close to zero at the boundary so that a negligible amount of energy exits the system due to the impedance boundary conditions in a single iteration. These two defining characteristics of the initial condition lead to the norm estimate of the fixed-point iteration operator \(S\) on the right of Figure 1. We observe that the norm of \(S\) does indeed approach unity at a rate of \(\omega^{-2}\), as predicted by theory. Thus, while the preceding analysis “artificially” leveraged energy conserving boundary conditions to obtain an estimate of the convergence rate for open problems, it is possible to realize the ‘worst-case’ rate implied by the energy conserving regime.

Remark 6.1. We note that the estimate for the convergence rate is a pointwise estimate. Repeated application of the fixed-point iteration will (eventually) remove the modes close to resonance and a faster convergence rate is observed. In Figure 2 we repeat the above experiment for the frequencies \(\omega = 10\pi, 40\pi,\) and \(70\pi\) but continue the iteration until the iterates converge to the zero solution. We observe that after an initial phase the rate of convergence of the iterates to the solution increases significantly since the data has propagated and exited the domain. We believe that the average behavior over many fixed-point iterations leads to the much more attractive rates seen in the Krylov-accelerated numerical experiments of [5]. Moreover, this example was pathologically constructed and we note that so far we have been unable to construct initial conditions to realize the worst-case rate in higher than one dimension.
Assuming radially symmetric solutions to the Helmholtz equation, it is possible to cast higher dimensional problems as 1D problems. We now consider solving an analogous problem in cylindrical (2D) and spherical (3D) coordinates with radial coordinate \( r \). We use a second order finite difference discretization (see [27] for details) on the unit ball, \( r \in [0,1] \), with an impedance boundary condition at \( r = 1 \). The initial condition is similar to the previous example,

\[
v_0(r) = \sin(\omega(r + 1)) - \frac{1}{2}(\sin((\omega + 2\pi)(r + 1)) + \sin((\omega - 2\pi)(r + 1))),
\]

\[
v_1(r) = -\frac{d}{dr}v_0(r).
\]

We consider a set of frequencies \( 10\pi, 11\pi, \ldots, 30\pi \) and use fifty points per wavelength in the computation with a CFL of \( 10^{-2} \). Below we show the results of the experiment. From the left of Figure 3 we observe that the norm of \( S \) approaches unity at a nearly linear rate in the frequency \( \omega \) in 2D and a sublinear rate for the 3D problem, both of which are more favorable than the quadratic rate in a single spatial dimension.

**Remark 6.2.** From the left of Figure 3 it is clear that with a fixed discretization and initial condition, the convergence rate improves with increasing dimension. This is perhaps unsurprising given an increase in the local energy decay rate for the wave equation from two to three dimensions, along with a richer set of directions in which waves may propagate and leave the domain.

### Time Discretization

We consider solving the Helmholtz equation with \( c = 1 \) and constant exact solution

\[
u(x) = 1, \quad 0 \leq x \leq 1.
\]

We take the frequency to be \( \omega = 1 \) and consider Dirichlet boundary conditions. We discretize the Laplacian with the standard three-point finite difference stencil and note that there is no error (aside from truncation errors) in the solution by a direct solution of the discrete Helmholtz equation. We use a centered modified equation time-stepping scheme of both second and fourth order, with both the original frequency and a modified frequency \( \tilde{\omega} \) with corresponding quadrature to
remove time discretization errors. We use the WaveHoltz iteration as a fixed-point iteration with a convergence criterion that the relative $L_2$ norm between successive iterations is smaller than $10^{-13}$. Using the original frequency in the calculation, we see on the right of Figure 3 that the WaveHoltz solution converges to the discrete Helmholtz solution with the same order as that of the time-step scheme used. With the modified frequency and quadrature, however, we see that the WaveHoltz iteration converges to the discrete Helmholtz solution up to roundoff errors.

Remark 6.3. While only centered time-stepping schemes are presented here, this approach can be extended to arbitrary time-steppers. A careful discrete analysis of the iteration isolated to a single eigenmode of the wave solution reveals what the modified frequency should be, and a modified quadrature as outlined above removes the time discretization error from the converged WaveHoltz solution. Thus, the choice of a time-stepper need not need be restricted to have the same order as the spatial discretization. With a corrected scheme it may be more advantageous to take as large a time-step as possible with a low order time-stepper.

6.1.3. Convergence Rate for Damped Helmholtz Equations. To study how the number of iterations scale with the Helmholtz frequency $\omega$ we solve the wave equation on the domain $x \in [-6,6]$ with constant wave speed $c^2(x) = 1$ and with a forcing

$$f(x) = \omega^2 e^{-(\omega x)^2},$$

that results in the solution being $O(1)$ for all $\omega$. We discretize using the energy based DG method discussed above and use upwind fluxes which adds a small amount of dissipation. We keep the number of degrees of freedom per wave length fixed by letting the number of elements be $5|\omega|$. We always take the polynomial degree to be 7, the number of Taylor series terms in the time-stepping to be 6, and use WHI accelerated by GMRES without restarts.

We report the number of iterations it takes to reach a GMRES residual smaller than $10^{-10}$ for the six possible combinations of Dirichlet, Neumann and impedance

![Figure 3. Left: The estimate of the quantity $1 - \|S\|$ with increasing Helmholtz frequency $\omega$ for a radially symmetric initial condition. Right: Convergence of the discrete WaveHoltz solution to the true solution of the discrete Helmholtz problem with fixed spatial discretization. The curves labeled with $\tilde{\omega}$ indicate the solution using the modified quadrature (4.8).](image-url)
boundary conditions for 200 frequencies distributed evenly from 1 to 100. The results for three levels of damping are displayed in Figure 4. On the left and middle of Figure 4 are damping parameters of $1/2\omega$ and $1/2$ respectively, from which it is clear that the scaling is sub-linear with increasing frequency. On the right in Figure 4 are results from a damping parameter that grows with frequency, $\omega/2$, which demonstrates a number of iterations that is both frequency independent and modest for a given GMRES tolerance. Interestingly, in this case the curve for each set of boundary conditions collapses to the same curve so that the iteration is insensitive to boundary conditions for a sufficiently large damping parameter.

![Figure 4. Number of iterations as a function of $\omega$ for different boundary conditions and damping parameters. Left to right: $\eta = 1/2\omega$, $1/2$, and $\omega/2$. Each legend entry indicates either Dirichlet (D), Neumann (N), or impedance (I) boundary conditions; the first letter at $x = -6$, and the second letter at $x = 6$.](image)

**Remark 6.4.** As seen in the prequel [5], the impedance-impedance conditions take the fewest iterations to reach convergence for lower levels of damping. We point out the preceding analysis assumes energy conserving boundary conditions to obtain estimates on the convergence rate of WaveHoltz as a fixed-point iteration. A different approach without the need for a Laplacian with a point-spectrum is needed to obtain rates depending on the specific boundary conditions.

6.2. **Examples in Two Dimensions.** In this section we present experiments in two space dimensions. For the following examples, we consider solving the Helmholtz equation for the wedge model which we adapt from [12, 29]. The domain is the rectangle $[0, 600] \times [0, 1000]$ with the (discontinuous) speed of sound $c(x) = \begin{cases} c_1 = 2100, & y \leq x/6 + 400, \\ c_2 = 1000, & x/6 + 400 \leq y \leq 800 - x/3, \\ c_3 = 2900, & \text{else}. \end{cases}$

On the boundary of the rectangle we impose the impedance boundary condition $w_t + c\nabla w \cdot \vec{n} = 0$. For the spatial discretization we use the SIPDG method with a penalty parameter choice of $\gamma = (p+1)^2$, where $p = 4$ is the polynomial order used in each element which results in a fifth order method. We discretize the domain with a total of 7680 triangular elements with a total of 115200 degrees of freedom. In time we use a fourth order Taylor method for time-stepping. For each example, we use the point-source

$$f(x,y) = \omega^2 \delta(|x - x_0|)\delta(|y - y_0|),$$
where \( x_0 = 300, y_0 = 0, \) \( \omega \) is the Helmholtz frequency, and \( \delta(z) \) is the usual Dirac delta function. These examples were implemented in the MFEM finite element discretization library [1].

6.2.1. Convergence for Damped Helmholtz Equations. We again study how the number of GMRES accelerated WHI iterations scale with the Helmholtz frequency \( \omega \) for the exemplary wedge problem.

We report the number of iterations it takes to reach a GMRES residual smaller than \( 10^{-10} \) for the frequencies \( 1, 2, \ldots, 100 \), with damping \( \eta = \omega/2 \) with either impedance or Neumann conditions on all sides of the rectangular domain.

![Figure 5](image_url)

**Figure 5.** Number of iterations to reach a GMRES tolerance of \( 10^{-10} \) for the wedge problem in 2D with all Neumann or all impedance boundary conditions.

The results for this experiment are shown in Figure 5, from which it is clear that the number of iterations is essentially independent of frequency for larger frequencies as was the case in a single spatial dimension. We again note that energy conserving boundary conditions require more iterations than the impedance case even in the presence of damping.

For a final example, in Figure 6 we display the solution of the damped (and undamped) Helmholtz equation using the GMRES accelerated WHI for a frequency of \( \omega = 40\pi \) with damping \( \eta = \omega/2 \) and 0, respectively.

7. Summary and Future Work

We have presented and extended analysis of the WaveHoltz iteration, an iterative method for solving the Helmholtz equation, applied to wave equations with and without damping. The general iteration has the same rate of convergence as the energy conserving case presented in [5], but is a more general and appropriate formulation for considering problems with impedance/Sommerfeld boundary conditions. For problems with damping, the WaveHoltz iteration always converges and numerical experiments verify the frequency independent convergence of problems with sufficient levels of damping.

We have provided analysis of the interior impedance problem in a single dimension and constructed an example in which the worst-case convergence rate is realized, despite the numerical results of our previous paper indicating much more
favorable scaling for non-energy conserving boundary conditions. We have additionally investigated higher order modified equation time-stepping schemes and shown that the WaveHoltz solution converges to the discrete Helmholtz solution to the order matching the order of the chosen time-stepping scheme. In addition, we have presented a method to completely remove time-discretization error for centered modified equation time-stepping schemes.

Finally, here we have only considered acoustic wave propagation. In future work we hope to apply the WaveHoltz iteration to elastic problems. Moreover, we have not yet tried to leverage sweeping preconditioner ideas here and hope to study the numerical and theoretical properties of these in the future.

APPENDIX A. PROOF OF LEMMA 2.2

We show the results for the rescaled function

$$\gamma(r) := \gamma(r\omega) = \frac{2}{T} \int_0^T \left( \cos(\omega t) - \frac{1}{4} \right) \sin(r\omega t) \, dt$$

$$= \frac{1}{\pi} \int_0^{2\pi} \left( \cos(t) - \frac{1}{4} \right) \sin(rt) \, dt.$$
By direct integration we get

\[ \bar{\gamma}(r) = \frac{1}{\pi} \int_0^{2\pi} \frac{1}{2} \left( \sin((r+1)t) + \sin((r-1)t) \right) - \frac{1}{4} \sin(rt) \, dt \]

\[ = \frac{(1 + 3r^2) \sin^2(\pi r)}{2\pi r(r^2 - 1)} \]

\[ = \frac{\pi r(1 + 3r^2) \text{sinc}(r/2)}{2(r^2 - 1)}, \]

where

\[ \text{sinc}(r) = \frac{\sin(2\pi r)}{2\pi r}. \]

From [5] we have the following expression for \( \beta \):

\[ \bar{\beta}(r) = \frac{1}{\pi} \int_0^{2\pi} \frac{1}{2} \left( \cos((r+1)t) + \cos((r-1)t) \right) - \frac{1}{4} \cos(rt) \, dt = \frac{(1 + 3r^2) \sin(2\pi r)}{4\pi r(r^2 - 1)} = \frac{(1 + 3r^2) \text{sinc}(r)}{2(r^2 - 1)}. \]

Then the eigenvalues of the WaveHoltz operator applied to the first order system are

\[ |\bar{\mu}(r)|^2 = \beta^2(r) + \bar{\gamma}^2(r) = \frac{(1 + 3r^2)^2 \sin^2(\pi r)}{4\pi^2 r^2(r^2 - 1)^2} = \frac{(1 + 3r^2)^2 \text{sinc}^2(r/2)}{4(r^2 - 1)^2}. \]

We now first consider \( 0 \leq r \leq 0.5 \) and note that \( |\mu(r)|^2 \) is a positive, increasing function on this interval so that

\[ |\bar{\mu}(r)|^2 \leq |\bar{\mu}(1/2)| = \frac{49}{9\pi^2} \leq 0.56. \]

For \( 1/2 \leq r \leq 3/2 \) we instead center around \( r = 1 \) and get for \( |\delta| \leq 1/2, \)

\[ |\bar{\mu}(1 + \delta)|^2 = \frac{(3(\delta + 1)^2 + 1)^2 \sin^2(\pi \delta)}{4\pi^2 \delta^2(1 + \delta)^2(2 + \delta)^2} = \frac{(3(\delta + 1)^2 + 1)^2 \text{sinc}^2(\delta/2)}{4(1 + \delta)^2(2 + \delta)^2}. \]

We use the fact that \( \sin(x) \leq x - \tilde{\alpha}x^3 \) in the interval \( x \in [0, \pi] \) for any \( \tilde{\alpha} \in [0, \pi^{-2}] \).

This leads to the following estimate for the sinc function

\[ 0 \leq \text{sinc}(r/2) \leq 1 - \alpha r^2, \quad r \in [-0.5, 0.5], \quad \alpha \in [0, 1]. \]

Using (A.1) with \( \alpha = 1 \), gives

\[ |\bar{\mu}(1 + \delta)|^2 \leq \frac{(3(\delta + 1)^2 + 1)^2(1 - \delta^2)^2}{4(1 + \delta)^2(2 + \delta)^2} = \frac{(4 + 2\delta - 3\delta^2 - 3\delta^3)^2}{4(2 + \delta)^2} \leq \frac{(4 + 2\delta - 2\delta^2 - \delta^3)^2}{4(2 + \delta)^2} = \frac{1 - \delta^2}{2}^2 = 1 - \delta^2 + \frac{\delta^4}{4} \leq 1 - \frac{15}{16}\delta^2, \]
since \( |\delta| < 1/2 \). A Taylor expansion around \( \delta = 0 \) for \( |\delta| \leq 1/2 \) immediately gives the bound
\[
\sqrt{1 - \delta^2} \leq 1 - \frac{\delta^2}{2} \implies |\mu(1 + \delta)| \leq \sqrt{1 - \frac{15}{16} \delta^2} \leq 1 - \frac{15\delta^2}{32}.
\]
If we consider \( r \geq 3/2 \),
\[
|\bar{\mu}(r)|^2 = \frac{(1 + 3r^2)^2 \sin^2(\pi r)}{4(r^2 + 1)^2} \leq \frac{(1 + 3r^2)^2}{4(r^2 + 1)^2},
\]
which is a positive and decreasing function. It follows that
\[
|\bar{\mu}(r)|^2 \leq \frac{(1 + 3(3/2)^2)^2}{4((3/2)^2 - 1)^2} \leq 0.44,
\]
for \( r \geq 3/2 \). Finally, for a more general bound for \( r > 1 \) we have \( 1/(r+1) - 1/2r \geq 0 \) so that
\[
|\bar{\mu}(r)|^2 = \frac{(1 + 3r^2)^2 \sin^2(\pi r)}{4\pi^2r^2(r^2 - 1)^2} \leq \frac{(1 + 3r^2)^2}{4\pi^2r^2(r^2 - 1)^2} = \frac{1}{\pi^2} \left( \frac{1}{r + 1} + \frac{1}{r - 1} - \frac{1}{2r} \right)^2 \leq \left( \frac{3}{2\pi(r - 1)} \right)^2,
\]
which gives
\[
|\bar{\mu}(r)| \leq \frac{3}{2\pi(r - 1)}.
\]
To prove (2.13), we use a Taylor expansion of \( \bar{\mu}(r) \) about \( r = 1 \) in the interval \( r \in (1/2, 3/2) \),
\[
|\bar{\mu}(1 + \delta)| = 1 + \frac{\delta^2}{2} \frac{d^2}{dr^2} |\bar{\mu}(r)|_{r=1} + \frac{\delta^3}{6} \bar{R}(\delta),
\]
where \( \bar{R}(\delta) \) is the remainder term. We note that by product rule we have
\[
\frac{d}{dr} |\bar{\mu}(r)| = \frac{1}{|\bar{\mu}|} (\bar{\beta} \bar{\beta}' + \bar{\gamma} \bar{\gamma}').
\]
Since
\[
\frac{d}{dr} |\bar{\mu}(r)|^{-s} = -s |\bar{\mu}(r)|^{-s-1} \frac{d}{dr} |\bar{\mu}(r)| = \frac{-s}{|\bar{\mu}(r)|^{s+2}} (\bar{\beta} \bar{\beta}' + \bar{\gamma} \bar{\gamma}'),
\]
by repeated product rule we can then show that
\[
\frac{d^3}{dr^3} |\bar{\mu}(r)| = \frac{3}{|\bar{\mu}|^5} (\bar{\beta} \bar{\beta}' + \bar{\gamma} \bar{\gamma}')^2 - \frac{1}{|\bar{\mu}|^3} (\bar{\beta} \bar{\beta}'' + (\bar{\beta}')^2 + \bar{\gamma} \bar{\gamma}'' + (\bar{\gamma}')^2)(1 + \bar{\beta} \bar{\beta}' + \bar{\gamma} \bar{\gamma}')
\]
\[+ \frac{1}{|\bar{\mu}|} (\bar{\beta} \bar{\beta}''' + 3\bar{\beta}' \bar{\beta}'' + \bar{\gamma} \bar{\gamma}''' + 3\bar{\gamma}' \bar{\gamma}'').
\]
We note that \( |\bar{\mu}(r)| \geq |\bar{\mu}(3/2)| \geq 1/\pi \) in the interval \( 1/2 \leq r \leq 3/2 \), and that we have the following bound
\[
\sup_{r \geq 0} |\bar{\beta}^{(s)}(r)| \leq \frac{1}{\pi} \int_0^{2\pi} t^s \left( 1 + \frac{1}{4} \right) dt = \frac{2^{s-1} \pi^s}{s+1}.
\]
which similarly holds for \( \sup_{r \geq 0} |\tilde{\gamma}^{(s)}(r)| \) for \( s = 0, 1, 2, \ldots \). Thus by Taylor’s theorem we have

\[
|\tilde{R}(\delta)| \leq \sup_{1/2 \leq r \leq 3/2} \left| \frac{d^3}{dr^3} |\tilde{\mu}(r)| \right|
\]

\[
\leq \frac{3}{4} \frac{25^2 \pi^2}{4} + \frac{3}{4} \frac{25 \pi^2}{4} \left( \frac{50 \pi^2}{3} + \frac{25 \pi^2}{2} \right) \left( 1 + \frac{25 \pi}{2} \right) + 3 \cdot 75 \pi^2
\]

\[
= \frac{25 \pi^4}{4} \left( 36 + 20 \pi + 250 \pi^2 + 75 \pi^3 \right).
\]

Then, \( |R(\delta)| \leq |\tilde{R}(\delta)|/6. \) Finally,

\[
\frac{d^2}{dt^2} [||\tilde{\mu}(r)||]_{r=1} = \frac{1}{6} (3 - 2 \pi^2) = -2b_1.
\]

**APPENDIX B. WAVE EQUATION EXTENSION**

Let \( \Omega = (-\infty, 0) \) and let \( f \in L^2(\Omega) \) be compactly supported in \( \Omega \) away from \( x = 0 \). Additionally, assume \( 1/c^2 \in L^1_{\text{loc}}(\Omega) \) with \( c(0) = c_0 \) on the interval \([-\delta, 0)\) for some \( \delta > 0 \). We consider the semi-infinite problem

\[
\begin{align*}
\frac{\partial w}{\partial t} &= \frac{\partial}{\partial x} \left[ c^2(x) \frac{\partial}{\partial x} w \right] - \text{Re} \{ f(x)e^{i\omega t} \}, \quad x \leq 0, \quad 0 \leq t \leq T, \\
w(0, x) &= v_0(x), \quad w_t(0, x) = v_1(x), \\
aw_t(t, 0) + \beta c_0 w_x(t, 0) &= 0.
\end{align*}
\]

Let \( \tilde{w} \) solve the extended wave equation

\[
\begin{align*}
\frac{\partial \tilde{w}}{\partial t} &= \frac{\partial}{\partial x} \left[ c^2(x) \frac{\partial}{\partial x} \tilde{w} \right] - \text{Re} \{ \tilde{f}(x)e^{i\omega t} \}, \quad x \in \mathbb{R}, \quad 0 \leq t \leq T, \\
\tilde{w}(0, x) &= \tilde{v}_0(x), \quad \tilde{w}_t(0, x) = \tilde{v}_1(x), \\
a\tilde{w}_t(t, 0) + \beta c_0 \tilde{w}_x(t, 0) &= 0,
\end{align*}
\]

where \( \tilde{f} \) is a zero extension, \( \tilde{c} \) is the extended wavespeed

\[
\tilde{c}(x) = \begin{cases} 
    c_0, & -\delta < x \leq 0, \\
    \tilde{c}_0, & x > 0,
\end{cases}
\]

and (I) \( \tilde{v}_0 \in H^1(\mathbb{R}) \) and \( \tilde{v}_1 \in L^2(\mathbb{R}) \) are extensions of the initial data. We choose the extensions of \( v_0 \) and \( v_1 \) such that

\[
\tilde{v}_1(x) + \tilde{v}_0(x) = 0, \quad x > 0, \quad (\text{II})
\]

so that the wave solution in the region \( x > 0 \) satisfies the condition \( w_t + w_x = 0 \) at \( x = 0 \), ensuring no data propagates into the original domain \( x < 0 \). In particular, we may take \( \tilde{v}_0 \) to be constant and \( \tilde{v}_1 \equiv 0 \). Moreover, since \( c \) is constant in \([-\delta, 0] \), the solution will then be of the form

\[
\tilde{w}(t, x) = \begin{cases} 
    w_L(x + c_0 t) + w_R(x - c_0 t), & -\delta \leq x \leq 0, \\
    w_T(x - \tilde{c}_0 t), & x > 0,
\end{cases}
\]
for some functions \( w_L, w_R, \) and \( w_T \). At \( x = 0 \) where \( \tilde{c} \) is (potentially) discontinuous, the weak solution satisfies the interface conditions that \( \tilde{w} \) and \( \tilde{c}^2 \tilde{w}_x \) are both continuous. These requirements lead to the relations

\[
\begin{align*}
   w_L(c_0 t) + w_R(-c_0 t) &= w_T(-\tilde{c}_0 t), \\
   \tilde{c}_0^2 (w'_L(c_0 t) + w'_R(-c_0 t)) &= \tilde{c}_0^2 w'_T(-\tilde{c}_0 t).
\end{align*}
\]

It follows that

\[
\tilde{w}_t(t, 0^-) = c_0 (w'_L(c_0 t) - w'_R(-c_0 t)) = -\tilde{c}_0 w'_T(-\tilde{c}_0 t), \quad c_0 \tilde{w}_x(t, 0^-) = \frac{\tilde{c}_0^2}{c_0} w'_T(-\tilde{c}_0 t),
\]

so that the impedance condition

\[
\alpha \tilde{w}_t(t, 0^-) + \beta c_0 \tilde{w}_x(t, 0^-) = \left( -\alpha \tilde{c}_0 + \beta \frac{\tilde{c}_0^2}{c_0} \right) w'_T(-\tilde{c}_0 t) = 0,
\]

is satisfied if

\[
\tilde{c}_0 = \frac{\alpha}{\beta} c_0. \tag{III}
\]

With this choice of the extended wavespeed \( \tilde{c}_0 \), both \( \tilde{w} \) and \( w \) satisfy the same PDE and condition at \( x = 0 \) so that they must be equal for \( x < 0 \). In summary, if we have that conditions (I-III) are satisfied, we have that \( \tilde{w}(t, x) = w(t, x) \) for \( x < 0 \).

We note that a similar argument can be made for an interior impedance problem on a bounded domain, \( a \leq x \leq b \), to a problem on \( \mathbb{R} \). In this case, assuming \( c(a) = c_a, c(b) = c_b \) where \( c \) is constant near the endpoints, then the following problem has \( \tilde{w}(t, x) = w(t, x) \) for \( a \leq x \leq b \):

\[
\begin{align*}
   \tilde{w}_t &= \frac{\partial}{\partial x} \left[ \tilde{c}_0^2(x) \frac{\partial}{\partial x} \tilde{w} \right] - \text{Re}\{ \tilde{f}(x)e^{-i\omega t} \}, \quad x \in \mathbb{R}, \quad 0 \leq t \leq T, \\
   \tilde{w}(0, x) &= \tilde{v}_0(x), \quad \tilde{w}_t(0, x) = \tilde{v}_1(x),
\end{align*}
\]

where \( \tilde{v}_0 \) and \( \tilde{c} \) are the constant extensions (with \( \gamma = \alpha/\beta \))

\[
\tilde{v}_0(x) = \begin{cases} 
   v_0(a_0), & x < a, \\
   v_0(x), & a \leq x \leq b, \\
   v_0(b_0), & b < x,
\end{cases} \quad \tilde{c}(x) = \begin{cases} 
   \gamma c_a, & x < a, \\
   c(x), & a \leq x \leq b, \\
   \gamma c_b, & b < x,
\end{cases}
\]

and \( \tilde{v}_1, \tilde{f} \) are zero extensions of \( v_1 \) and \( f \), respectively.

Since the solutions to the wave equation have finite speed of propagation, we may replace the domain \( \mathbb{R} \) for \( \tilde{w} \) by a large enough domain with any boundary condition given that any reflections at the new boundary do not re-enter the region \( a \leq x \leq b \). Let \( \tilde{a} < a - c_a T/2 \) and \( \tilde{b} > b + c_b T/2 \). We define the extension operator \( E \) such that \([v_0, v_1]^T \to [\tilde{v}_0, \tilde{v}_1]^T\) where \( \tilde{v}_0 \) and \( \tilde{c} \) are the extensions as above and \( \tilde{v}_1, \tilde{f} \) are zero extensions of \( v_1 \) and \( f \), respectively. We now consider the (finite interval) extended problem with homogeneous Neumann conditions

\[
\begin{align*}
   \tilde{w}_t &= \frac{\partial}{\partial x} \left[ \tilde{c}_0^2(x) \frac{\partial}{\partial x} \tilde{w} \right] - \text{Re}\{ \tilde{f}(x)e^{-i\omega t} \}, \quad \tilde{a} \leq x \leq \tilde{b}, \quad 0 \leq t \leq T, \\
   \tilde{w}(0, x) &= \tilde{v}_0(x), \quad \tilde{w}_t(0, x) = \tilde{v}_1(x), \\
   \tilde{w}_x(t, \tilde{a}) &= 0, \quad \tilde{w}_x(t, \tilde{b}) = 0.
\end{align*}
\]
Defining the projection operator $P$ as the restriction of $\tilde{w}$ to $a \leq x \leq b$ then it follows that $P\tilde{w} = w$ where $w$ is the original wave solution to the interior impedance problem.

**APPENDIX C. WELL-DEFINEDNESS OF MODIFIED FREQUENCIES**

Here we show that the modified frequency $\tilde{\omega}$ is well-defined. This is given by the following lemma.

**Lemma C.1.** For each $\omega \in \mathbb{R}$ satisfying $0 < \Delta t \omega \leq 1$ there is a modified frequency $\tilde{\omega} \in \mathbb{R}$ which is the smallest positive real number satisfying

$$\sin^2(\omega \Delta t/2) = \sum_{j=1}^{m} \frac{(-1)^{j+1} (\Delta t \tilde{\omega})^{2j}}{2(2j)!}. \tag{C.1}$$

Moreover, there is a constant $C_m < 1$ that only depends on $m$ such that

$$0 < \Delta t \tilde{\omega} \leq 2, \quad |\omega - \tilde{\omega}| \leq C_m \Delta t^{2m} \omega^{2m+1}, \quad C_m := 5/(2m + 2)!$$

and for all $0 \leq \Delta t \lambda \leq 2$, it holds that

$$\left| \sum_{j=1}^{m} \frac{(-1)^{j+1} (\Delta t \lambda)^{2j}}{2(2j)!} \right| \leq 1. \tag{C.3}$$

**Proof.** We define the polynomial

$$p(x) = \sum_{j=1}^{m} \frac{(-1)^{j+1} x^j}{2(2j)!} - \sin^2(\omega \Delta t/2), \tag{C.4}$$

and note that $(\Delta t \tilde{\omega})^2$ is a root of $p(x)$. On the interval $[0, 1/2]$ we have that $\sin^2(x)$ is increasing so that

$$0 < \sin^2(\omega \Delta t/2) \leq \sin^2(1/2) \leq 0.23 < 1,$$

immediately giving $p(0) < 0$. Moreover,

$$p(4) = \frac{1}{2} \sum_{j=1}^{m} \frac{(-1)^{j+1} 2^2j}{(2j)!} - \sin^2(\omega \Delta t/2)$$

$$= \frac{1}{2} \sum_{j=1}^{\infty} \frac{(-1)^{j+1} 2^2j}{(2j)!} + \frac{1}{2} \sum_{j=m+1}^{\infty} \frac{(-1)^{j+1} 2^2j}{(2j)!} - \sin^2(\omega \Delta t/2)$$

$$= \sin^2(1) + \frac{1}{2} \sum_{j=m+1}^{\infty} \frac{(-1)^{j+1} 2^2j}{(2j)!} - \sin^2(\omega \Delta t/2). \tag{C.5}$$

We note that,

$$\sum_{j=2}^{\infty} \frac{2^2j}{(2j)!} = \sum_{j=0}^{\infty} \frac{2^2j}{(2j)!} - 3 = \cosh(2) - 3,$$

so that

$$\left| \frac{1}{2} \sum_{j=m+1}^{\infty} \frac{(-1)^{j+1} 2^2j}{(2j)!} \right| < \frac{1}{2} \sum_{j=m+1}^{\infty} \frac{2^2j}{(2j)!} \leq \frac{1}{2} \sum_{j=2}^{\infty} \frac{2^2j}{(2j)!} = \frac{1}{2}(\cosh(2) - 3). \tag{C.6}$$
Since also $\sin^2(\omega \Delta t/2) \leq \sin^2(1/2)$, we get

$$p(4) > \sin^2(1) - \frac{1}{2} (\cosh(2) - 3) - \sin^2(1/2) \approx 0.097 > 0.$$  

By the intermediate value theorem, it follows that $p(x)$ has a root in the interval $(0, 4)$. We next need to show that $p'(x) \neq 0$ on this interval to guarantee the root is unique. Taking a derivative,

$$\frac{d}{dx} p(x) = \sum_{j=1}^{m} \frac{(-1)^{j+1} x^j}{(2j)!} = \frac{1}{2} \left[ 1 + \sum_{j=2}^{m} \frac{(-1)^{j+1} x^{j-1}}{(2j-1)!} \right].$$

We then have

$$\sum_{j=2}^{m} \frac{(-1)^{j+1} x^{j-1}}{(2j-1)!} \geq - \sum_{j=2}^{m} \frac{2^{j-1}}{(2j-1)!} = - \frac{1}{\sqrt{2}} \sum_{j=2}^{m} \frac{\sqrt{2}^{j-1}}{(2j-1)!} \geq - \frac{1}{\sqrt{2}} \left[ \sum_{j=1}^{\infty} \frac{\sqrt{2}^{j-1}}{(2j-1)!} - \sqrt{2} \right] = - \frac{\sinh(\sqrt{2})}{\sqrt{2}} + 1,$$

so that

$$(C.7) \quad \frac{d}{dx} p(x) = \frac{1}{2} \left[ 1 + \sum_{j=2}^{m} \frac{(-1)^{j+1} x^{j-1}}{(2j-1)!} \right] \geq \frac{1}{2} - \frac{\sinh(\sqrt{2})}{\sqrt{2}} + 1 > \frac{1}{10} > 0.$$  

This gives that there is a unique, positive, real-valued $\bar{\omega}$ with $0 < \Delta t \bar{\omega} < 2$ that satisfies the relation (C.1), showing the first part of the lemma. For the last part we let $x = \Delta t \bar{\omega} \in (0, 1]$, $\bar{x} = \Delta t \bar{\omega} \in (0, 2)$, and $R_m = p(x^2) - p(\bar{x}^2)$ where $p(x)$ is defined as in (C.4). By the mean value theorem we have

$$|R_m| = |p(x^2) - p(\bar{x}^2)| = |(x^2 - \bar{x}^2)p'(\xi)| = |x - \bar{x}| |x + \bar{x}| |p'(\xi)|,$$

for some $\xi \in (0, 2)$, so that

$$|x - \bar{x}| \leq \frac{|R_m|}{|x + \bar{x}| |p'(\xi)|}.$$

Since $\bar{x}^2$ is a root of $p$, a Taylor series estimate gives

$$|R_m| = |p(x^2)| = \sum_{j=1}^{m} \frac{(-1)^{j+1} x^j}{2(2j)!} - \sin^2(\omega \Delta t/2) = \left| \sum_{j=m+1}^{\infty} \frac{(-1)^{j+2} (\Delta t \omega)^{2j}}{2(2j)!} \right| \leq \frac{(\Delta t \omega)^{2m+2}}{2(2m+2)!},$$

which gives

$$|x - \bar{x}| \leq \frac{|R_m|}{|x + \bar{x}| |p'(\xi)|} \leq \frac{\Delta t^{2m+1} \omega^{2m+2}}{2(2m+2)! (\omega + \bar{\omega}) |p'(\xi)|} \Delta t^{2m} \omega^{2m+2} = \frac{\Delta t^{2m} \omega^{2m+2}}{2(2m+2)! (\omega + \bar{\omega}) |p'(\xi)|},$$

$$\implies |\omega - \bar{\omega}| \leq \frac{\Delta t^{2m} \omega^{2m+2}}{2(2m+2)! (\omega + \bar{\omega}) |p'(\xi)|}.$$
By (C.7) we have that $|p'(x)| > 1/10$ in $[0, 4]$, which finally gives

$$(C.8) \quad |\omega - \tilde{\omega}| \leq \frac{10\Delta t^{2m} \omega^{2m+2}}{2(2m+2)!(\omega + \tilde{\omega})} \leq \frac{5\Delta t^{2m} \omega^{2m+1}}{(2m+2)!} =: C_m \Delta t^{2m} \omega^{2m+1}.$$

We finally prove (C.3). It is trivially true for $\lambda = 0$ so we assume that $\lambda > 0$. We define $a_k = (\Delta t \lambda)^{2k}/2(2k)!$, and note that $a_{k+1}/a_k < 1$ so that $a_k > a_{k+1} > 0$ and that $a_1 = (\Delta t \lambda)^2/4 \leq 1$. Letting

$$\tilde{m} = \begin{cases} m, & m \text{ odd,} \\ m+1, & m \text{ even,} \end{cases}$$

then we have

$$\sum_{k=1}^{m} \frac{(-1)^{k+1} (\Delta t \lambda)^{2k}}{2(2k)!} = \sum_{k=1}^{\tilde{m}} (-1)^{k+1} a_k \leq \sum_{k=1}^{\tilde{m}} (-1)^{k+1} a_k
= a_1 - \sum_{k=1}^{(\tilde{m}-1)/2} (a_{2k} - a_{2k+1}) \leq a_1 \leq 1,$$

If instead

$$\tilde{m} = \begin{cases} m+1, & m \text{ odd,} \\ m, & m \text{ even,} \end{cases}$$

then we have the bound

$$\sum_{k=1}^{m} \frac{(-1)^{k+1} (\Delta t \lambda)^{2k}}{2(2k)!} = \sum_{k=1}^{\tilde{m}} (-1)^{k+1} a_k \geq \sum_{k=1}^{\tilde{m}} (-1)^{k+1} a_k
= \sum_{k=1}^{\tilde{m}/2} (a_{2k-1} - a_{2k}) > 0,$$

proving (C.3).

□

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