Improved Accuracy for the Helmholtz Equation in Unbounded Domains

Eli Turkel *
Department of Mathematics
Tel Aviv University
Tel Aviv, Israel

Charbel Farhat and Ulrich Hetmaniuk
Department of Aerospace Sciences
and Center for Aerospace Structures
University of Colorado at Boulder
Boulder, Colorado

Abstract

Based on properties of the Helmholtz equation we derive a new equation for an auxiliary variable. This reduces much of the oscillations of the solution leading to more accurate numerical approximations to the original unknown. Computations confirm the improved accuracy of the new models in both two and three dimensions. This also improves the accuracy when one wants the solution at neighboring wavenumbers by using an expansion in k. We examine the accuracy for both waveguide and scattering problems as a function of k, h and the forcing mode l. The use of local absorbing boundary conditions is also examined as well as the location of the outer surface as functions of k. Connections with parabolic approximations are analyzed.

*work done while visiting the University of Colorado at Boulder

1 Introduction

Preconditioning is a technique where the equation is multiplied by an approximation to the solution operator. This (hopefully) yields a new equation with better conditioning. In classical preconditioning the purpose is to improve the convergence rate of an iterative solver (see however [32]). In this study we use an extension of preconditioning to improve the accuracy of a numerical approximation. The solutions of the Helmholtz equation are difficult to calculate because they are highly oscillatory [34]. By removing much of this oscillatory behavior through the preconditioning the remaining problem is easier to treat on a coarse mesh. We stress that this preconditioning is physically motivated and so depends on the nature of the problem to be solved. We consider both waveguide and scattering problems. The preconditioning will be different for each of these cases and also depends on the number of dimensions. For any given preconditioning one can construct an example that will not be improved or even made worse by the preconditioner. However, these counterexamples will be of the class for which the preconditioner is not appropriate. We compare the accuracy of linear finite elements for the approximation of both the Helmholtz equation and the new formulation. We also check the effect on calculating the solution at neighboring wave numbers. We consider the accuracy in a waveguide not only as a function of k and h but also the mode l of the forcing boundary function. We will also check this dependence for scattering problems. We also study the effect of local absorbing boundary conditions in both two and three dimensions. In addition we evaluate the effect of the position of the outer boundary has on the accuracy of the approximation.

2 One Dimensional Equation

The Helmholtz equation in one dimension reduces to the ordinary differential equation

$$u_{xx} + k^2 u = 0. \tag{1}$$

This has solutions of the form $u = Ae^{ikx} + Be^{-ikx}$. We assume the waves move from left to right. The Sommerfeld radiation condition eliminates waves entering the domain from infinity and so $B = 0$. Thus, we are led to defining

a new variable $u = ve^{ikx}$. Thus, for this simple problem the only outgoing solution is v=constant. v solves the equation

$$v_{xx} + 2ikv_x = 0. \tag{2}$$

The Sommerfeld radiation condition

$$u'(x) - iku(x) = o(1), \quad x \to \infty$$

is replaced by

$$v'(x) = o(1), \quad x \to \infty$$

Note that (2) has a solution of the form $v = A + Be^{-2ikx}$ and so has oscillatory behavior. $B = 0$ only because of the Sommerfeld radiation condition. Hence, the improved smoothness of v is due to the combination of the equation and the far field boundary condition and so is a global property. Hence, an analysis of the behavior of methods, e.g. multigrid, for this problem must use a global analysis and not just a local modal analysis that ignores the far field boundary condition.

3 Waveguide Problem

We consider the two dimensional problem

$$u_{xx} + u_{yy} + k^2 u = 0, \qquad 0 < x < \infty, \quad 0 < y < 1 \tag{3}$$

with boundary conditions $u(0, y) = f(y)$, $u_y(x, 0) = u_y(x, 1) = 0$ and u outgoing at infinity. The Neumann conditions at the top and bottom can easily be replaced by other boundary conditions. We use Neumann conditions on the side walls because they are a natural boundary condition for the finite element method. The extension to three dimensional Cartesian coordinates is straightforward. By separation of variables the solution to (3) is

$$u(x, y) = \sum_{l<k} a_l e^{i\sqrt{k^2-l^2}x} \cos(ly) + \sum_{l>k} b_l e^{-\sqrt{l^2-k^2}x} \cos(ly) \quad . \tag{4}$$

l is a positive integer multiple of π

The first sum represents traveling waves and the second sum evanescent waves. By linearity it is sufficient to consider the inflow condition $u(0,y) = \cos(ly)$.

We assume that the main propagation of waves is in the positive x direction and that the waves in the y direction are principally standing waves. As in the one dimensional case we introduce the new variable v by

$$u = ve^{ikx} \quad . \tag{5}$$

The equation for v is

$$v_{xx} + v_{yy} + 2ikv_x = 0, \qquad 0 < x < \infty, \quad 0 < y < 1 \tag{6}$$

with boundary conditions $v(0,y) = f(y)$, $v_y(x,0) = v_y(x,1) = 0$ and ve^{ikx} outgoing at infinity. The outgoing condition is imposed at a finite location $x = L$ and every y by

$$v_x(L,y) - i\left(\sqrt{k^2 - l^2} - k\right) v(L,y) = 0$$

for each traveling mode and a similar condition for the evanescent modes. If $l = 0$ this reduces to a homogeneous Neumann condition as in one dimension. Hence, for the lowest mode $l = 0$ the solution v is constant. For a general traveling mode l we have $v = e^{i(\sqrt{1-\frac{l^2}{k^2}}-1)kx}\cos(ly)$. If $\frac{l}{k}$ is small then v is a much smoother function that u. For evanescent modes the new variable v does not help and one should use instead $u = ve^{-kx}$. Since the evanescent modes decay exponentially therefore, in many problems that contain both traveling and evanescent modes it is more important to treat the traveling modes correctly than the evanescent modes.

If we eliminate the higher derivative v_{xx} in (6) because it is small compared with $2ikv_x$ then we recover the parabolic equation given by [10, 30],

$$2ikv_x + v_{yy} = 0 \qquad 0 < x < \infty \quad 0 < y < 1 \quad . \tag{7}$$

Equation (6) has the disadvantage that one is solving an elliptic equation rather than a parabolic equation which can be marched in x. However, it has the advantage that no terms are ignored and so is more accurate than the

parabolic approximation. It is also more accurate (on the numerical level) than the original Helmholtz equation since we are solving for the smooth portion of the solution. Each mode of (6) depends on $e^{i(\sqrt{k^2-l^2}-k)x}\cos(ly)$. So v_{xx} is proportional to $(\sqrt{k^2-l^2}-k)^2$ which is small when $\frac{l}{k}$ and k are small. The parabolic equation (7) has the Sommerfeld radiation condition built in. This is an advantage since we do not need to implement an absorbing boundary condition at the exit. However, it cannot handle backscattering. The full equation (6) accounts for backscattering though it will be less accurate since the wavenumber for the backscattered wave is essentially doubled.

The solution to (7) is $v = e^{-i\frac{l^2}{2k}x}\cos(ly)$ compared with $e^{i(\sqrt{1-\frac{l^2}{k^2}}-1)kx}\cos(ly)$ for (6). Expanding the square root we see that the parabolized equation has a phase error, for the l-th mode, given by $\left(\sqrt{1-\frac{l^2}{k^2}}-1\right)k+\frac{l^2}{2k} \simeq -\frac{l^4}{8k^3}$. The parabolic approximation will be discussed in more detail in the last section.

3.1 Perfectly Matched Layers (PML)

For the Helmholtz equation one needs to impose a boundary condition at each surface. At the exit to the waveguide one needs to simulate the Sommerfeld radiation condition that no waves enter the physical domain from infinity. A popular way is to add an artificial layer and to solve the PML equations within this layer. This was first proposed by Berenger [7] for the time dependent Maxwell equations. This can also be applied to the Helmholtz equation (see for example [33]). This is given by

$$\frac{\partial}{\partial x}\left(\frac{1}{S}\frac{\partial u}{\partial x}\right)+S\frac{\partial^2 u}{\partial y^2}+Sk^2u=0 \qquad S(x)=1+\frac{\sigma(x)}{ik} \tag{8}$$

$\sigma = 0$ inside the physical waveguide so we recover the Helmholtz equation. In the artificial layer σ is an increasing function of x starting at zero to match the interior and reaching $\sigma_{\max}$ at the exit. Usually σ is chosen as a polynomial in the distance from the end of the waveguide. We can generalize our previous approach by taking

$$u = ve^{ik\int_0^x S} \tag{9}$$

As before this removes the oscillatory behavior. v satisfies the equation

$$\frac{\partial}{\partial x}\left(\frac{1}{S}\frac{\partial v}{\partial x}\right)+S\frac{\partial^2 v}{\partial y^2}+2ikS\frac{\partial v}{\partial x}=0 \tag{10}$$

3.2 Bands of k

In [15] Djellouli, Farhat and Tezaur present a method to solve the Helmholtz equation for a wave number $k + \Delta k$ given the calculated solution at wave number k. The basic idea is to expand $u(k + \Delta k)$ in a Taylor series in k. The higher derivatives of u with respect to k obey a Helmholtz equation with a forcing term that depends on lower order derivatives. Assuming an LU decomposition of the Helmholtz operator has been formed these subsequent Helmholtz equations are solved very efficiently. This Taylor series does not converge very well due to numerical inaccuracies in approximating the Helmholtz equation for the high order derivatives. This series can be accelerated by using a Padé series or the epsilon algorithm.

We will study the effect of using (5) and (6) on improving the convergence and accuracy of these expansions. In [15] they were mainly concerned with the efficiency of finding solutions for a band of wavenumbers given the solution at a given wavenumber. It is well known (see e.g. [6, 13, 3]) that the accuracy of second order (in L^2) finite element method depends on k^3h^2. Hence, the solution for high wave numbers can be prohibitively expensive since it requires an extremely fine mesh. We will investigate the use of (5) on the pollution error. We emphasize that this is not done for all possible solutions of the Helmholtz equation but only for those that are physically relevant e.g. the waveguide and scattering problems.

Consider the two dimensional waveguide problem for a single mode, i.e. equation (3) with $f(y) = \cos(ly)$, l an integer multiple of π. Define $u^{(n)} = \frac{1}{n!}\frac{\partial^n u}{\partial k^n}$. Then $u^{(n)}$ satisfies the equation [15]

$$u_{xx}^{(n)} + u_{yy}^{(n)} + k^2 u^{(n)} = -2ku^{(n-1)} - u^{(n-2)}, \qquad n \geq 1 \quad u^{(-1)} = 0 \tag{11}$$

with boundary conditions

$$u^{(n)}(0, y) = 0, \qquad u_y^{(n)}(x, 0) = u_y^{(n)}(x, 1) = 0$$

and for finite x and every y

$$u_x^{(n)}(x, y) - i\sqrt{k^2 - l^2}u^{(n)}(x, y) = i\sum_{m=1}^{n} \frac{1}{m!}\frac{\partial^m}{\partial k^m}\left(\sqrt{k^2 - l^2}\right) u^{(n-m)}(x, y)$$

Similarly, we define $v^{(n)} = \frac{1}{n!}\frac{\partial^n v}{\partial k^n}$. This satisfies

$$v_{xx}^{(n)} + v_{yy}^{(n)} + 2ikv_x^{(n)} = -2iv_x^{(n-1)}, \qquad n \geq 1 \tag{12}$$

with boundary conditions

$$v^{(n)}(0,y) = 0, \qquad v_y^{(n)}(x,0) = v_y^{(n)}(x,1) = 0$$

and for finite x and every y

$$v_x^{(n)}(x,y) - i\left(\sqrt{k^2-l^2} - k\right) v^{(n)}(x,y) = i\sum_{m=1}^{n} \frac{1}{m!}\frac{\partial^m}{\partial k^m}\left(\sqrt{k^2-l^2} - k\right) v^{(n-m)}(x,y)$$

To avoid the large sums in the Sommerfeld radiation condition for the higher modes we keep only two terms in the sum, i.e. those that depend on $u^{(n-1)}$ and $u^{(n-2)}$ and similarly for v.

3.3 Implementation

We now consider three ways to calculate $u(k+\Delta k)$. Each has advantages and disadvantages.

The first way is to solve (6) by one's favorite method. This requires an approximation for the first derivative. We note that iv_x is a self-adjoint operator. Hence, if done appropriately the approximation to the equation is Hermitian. However, the Sommerfeld radiation condition is complex symmetric and so the total problem of equation plus boundary condition has no symmetry. As we will see the first BGT approximation to the Sommerfeld condition for scattering leads to a problem which is Hermitian symmetric for the Dirichlet boundary valued problem. This alternative has the major advantage that we expect the basic approximation for v to be much more accurate than that for u (see result section).

When we consider the solution for nearby wavenumbers we have $u(k+\Delta k) = v(k+\Delta k)e^{i(k+\Delta k)x}$. Hence, once we use the expansion to find $v(k+\Delta k)$ we immediately know $u(k+\Delta k)$. In [15] they solved the waveguide problem only for the lowest mode $l = 0$, and so $u = e^{ikx}$ and $v = 1$. This implies that all the higher derivatives of v are zero and so the Taylor series collapses to

the first term which gives the exact answer. To avoid this triviality we shall show results for higher modes. Nevertheless, as long as $\frac{l}{k} << 1$ we expect accurate results and a fast convergence.

Nevertheless, this method has several disadvantages. First, it requires new coding. Second, the symmetry may be lost due to either the boundary conditions or difficulties with the approximation to the first derivative. Hence, we present an alternative to the direct solution of (6).

The second way is to solve the original equation for u and its derivatives. We then use (5) to calculate v and its derivatives in order to get a Taylor series for $v(k+\Delta k)$. This has the advantage that the approximation to the partial differential equations need not be changed. This implies that basic approximation for u is not being improved as it is when solving (6). It has the further disadvantage that the Taylor series for $v(k+\Delta k)$ is polluted by the larger discretization errors in the derivatives of u. As we shall see in the results section this option gives much better results than solving (11) and a Taylor series for u but not as good as solving (12).

We assume we are given u and $u^{(n)} = \frac{1}{n!}\frac{\partial^n u}{\partial k^n}$ and wish to find $v^{(n)} = \frac{1}{n!}\frac{\partial^n}{\partial k^n}(ue^{-ikx})$. One can evaluate this directly by the binomial formula. This becomes complicated for high derivatives. In addition directly evaluating the factorial is extremely inaccurate for large n. Instead we use a recursion formula to find $v^{(n)}$. We shall do this in two stages. First we find the n-th derivative of v and then account for the factorial. We assume we are given

$$v(x;k) = F(x,k)u(x;k) \qquad \text{and}$$
$$G(x,k) = \frac{\partial F}{\partial k} \diagup F \quad .$$

We will consider in this study three special cases

$$\begin{array}{lll} \text{Cartesian:} & F(x,k) = e^{-ikx} & G(x,k) = -ix \\ \text{Cylindrical:} & F(r,k) = \dfrac{1}{H_0^{(1)}(kr)} & G(r,k) = \dfrac{H_1^{(1)}(kr)}{H_0^{(1)}(kr)} r \simeq -ir + \dfrac{1}{2k} \\ \text{Spherical:} & F(r,k) = kre^{-ikr} & G(r,k) = -ir + \dfrac{1}{k} \end{array} \tag{13}$$

We also consider three simplifications of these

$$\begin{aligned} \text{Cartesian:} \quad & F(x,k) = e^{-ikx} && G(x,k) = -ix \\ \text{Cylindrical:} \quad & F(r,k) = \sqrt{r}e^{-ikr} && G(r,k) = -ir \\ \text{Spherical:} \quad & F(r,k) = re^{-ikr} && G(r,k) = -ir \end{aligned} \tag{14}$$

Note that for (14) G is independent of k. In the following we ignore the derivatives of G with respect to k either because (14) is used or else we use the more accurate (13) but ignore the higher derivatives as being negligible for large k. The Cartesian case is the same in both sets. We then have

$$u(k+\Delta k) = \frac{v(k+\Delta k)}{F(x,k+\Delta k)} = \frac{F(x,k)}{F(x,k+\Delta k)} \sum_{n=0}^{N} (\Delta k)^n \left[\frac{1}{F(x,k)\, n!} \frac{\partial^n v}{\partial k^n} \right]$$

Define w_n by $w_0 = u$ and

$$\begin{aligned} \frac{\partial v}{\partial k} &= F(x,k) \left[G(x,k) w_0 + \frac{\partial w_0}{\partial k} \right] = F(x,k) w_1 \\ \frac{\partial^n v}{\partial k^n} &= F(x,k) \left[G(x,k) w_{n-1} + \frac{\partial w_{n-1}}{\partial k} \right] = F(x,k) w_n \end{aligned} \tag{15}$$

So

$$\begin{aligned} w_1 &= G(x,k) w_0 + \frac{\partial w_0}{\partial k} \\ \frac{1}{n!} \frac{\partial^n w_1}{\partial k^n} &= G(x,k) \left(\frac{1}{n!} \frac{\partial^n w_0}{\partial k^n} \right) + (n+1) \left(\frac{1}{(n+1)!} \frac{\partial^{n+1} w_0}{\partial k^{n+1}} \right) \end{aligned} \tag{16}$$

More generally define

$$\begin{aligned} w_0^{(n)} &= \frac{1}{n!} \frac{\partial^n u}{\partial k^n} \\ w_p^{(n)} &= \frac{1}{n!} \frac{\partial^n w_p}{\partial k^n} \qquad n = 0, \ldots N-p \qquad p = 1, \ldots N \end{aligned} \tag{17}$$

Then from (16) and (17) we have

$$w_p^{(n)} = G(x,k) w_{p-1}^{(n)} + (n+1) w_{p-1}^{(n+1)} \qquad n = 0, \ldots N-p \qquad p = 1, \ldots N$$

Finally define $v_p^{(n)} = \frac{w_p^{(n)}}{p!}$. Then

$$v_p^{(n)} = \frac{G(x,k)v_{p-1}^{(n)} + (n+1)v_{p-1}^{(n+1)}}{p} \qquad n = 0, ...N-p \qquad p = 1, ...N \quad (18)$$

and

$$\frac{1}{p!}\frac{\partial^p v}{\partial k^p} = F(x,k)v_p^{(0)}. \quad (19)$$

Note that from (18) $v_p^{(0)}$ is computed recursively starting with $v_0^{(p)}$. So

$$\begin{aligned} u(k+\Delta k) &= \frac{F(x,k)}{F(x,k+\Delta k)} \sum_{n=0}^{N} (\Delta k)^n \left[\frac{1}{F(x,k)\, n!} \frac{\partial^n v}{\partial k^n} \right] \\ &= \frac{F(x,k)}{F(x,k+\Delta k)} \sum_{n=0}^{N} (\Delta k)^n v_n^{(0)} \ . \end{aligned} \quad (20)$$

The third alternative is to utilize the difference formula for v to construct a new difference formula for u. We shall illustrate this for the one dimensional equation. A standard second order difference (or linear finite element) approximation to (2) is

$$v_{j+1} - 2v_j + v_{j-1} + ikh(v_{j+1} - v_{j-1}) = 0$$

Substituting $v_j = e^{-ijkh}u_j$ and canceling the common factor of e^{-ijkh} we get

$$e^{-ikh}u_{j+1} - 2u_j + e^{ikh}u_{j-1} + ikh(e^{-ikh}u_{j+1} - e^{ikh}u_{j-1}) = 0$$

or

$$u_{j+1} - 2u_j + u_{j-1} + \left[e^{-ikh}(1+ikh) - 1\right] u_{j+1} + \left[e^{ikh}(1-ikh) - 1\right] u_{j-1} = 0$$

The basic approximation to the differential equation without considering the boundaries is again Hermitian symmetric. A Taylor series expansion shows that this is a second order approximation to the Helmholtz equation. By construction the formula is exact for $u = e^{ikx}$. However, it is not clear if

this can be represented as a Petrov-Galerkin method since we have only manipulated u and v and not the basis functions. As with the first approach this requires recoding the approximation to the partial differential equation. The Sommerfeld condition will be simplified as it was for the first approach. However, now a Neumann boundary condition at the inlet or scatterer presents no difficulty as it can be either a natural boundary condition within a finite element approach or any standard approximation to the normal derivative for the finite difference approach.

3.4 Dispersion Analysis

We have already shown that (6) is exact for the first mode, i.e. for one dimensional wave propagation. We next investigate the behavior of the various schemes for higher modes. Rather than have the modes excited by the boundary conditions it is easier to analyze the differential equation with a forcing term. In this case the speed of the numerical approximation is fixed by the forcing mode and the only error can be the amplitude of the wave not in its phase. When we consider the sum of waves the concept of phase is not clear. Consider $u = A_1 e^{ik_1 x} + A_2 e^{ik_2 x}$ by varying the amplitudes of A_1 and A_2 one change the phase of u between k_1 and k_2. Hence, amplitude and phase are distinct entities only for a single wave but not for a sum of waves. We are interested in the numerical approximation to

$$U_{xx} + k^2 U = (k^2 - m^2) e^{imx} \tag{21}$$

Boundary conditions are added so that the solution is $U = Ae^{imx}$ with $A = 1$. For a traveling wave we assume $k > m$. By comparison with (4) we choose $m^2 = k^2 - l^2$ where l is the mode number of the inlet boundary condition.

We begin with a second order finite difference approximation to the forced Helmholtz equation.

$$u_{j+1} - 2u_j + u_{j-1} + k^2 h^2 u_j = h^2 (k^2 - m^2) e^{imjh} \tag{22}$$

The solution is of the form $u = A_h e^{imjh}$. Substituting this into (22) we get

$$A_h = \frac{(k^2 - m^2)h^2}{k^2 h^2 - 2(1 - \cos(mh))} = \frac{l^2}{k^2 - \frac{2}{h^2}(1 - \cos(\sqrt{k^2 - l^2}h))}$$

expanding the cosine for small kh we have

$$A_h \sim \frac{(k^2-m^2)h^2}{(k^2-m^2)h^2 + m^4h^4/12} = \frac{1}{1+\frac{(k^2-l^2)^2h^2}{12l^2}}$$

At $l = k$ we have $A_h = 1$ and there is no error. As l decreases A_h decreases and the error in the amplitude increases.

We next consider the equation for $v = ue^{-ikx}$.

$$v_{j+1} - 2v_j + v_{j-1} + ikh(v_{j+1} - v_{j-1}) = -h^2(m^2 + 2km)e^{imjh} \tag{23}$$

Now $m = \sqrt{k^2 - l^2} - k$. The solution is again of the form $v = A_h e^{imjh}$. Substituting this into (23) we get

$$A_h = \frac{(m^2+2km)h^2}{2(1-\cos(mh)) + 2kh\sin(mh)}$$

expanding the sine and cosine we have

$$\begin{aligned} A - A_h &\sim 1 - \frac{(m^2+2km)h^2}{(m^2+2km)h^2 - m^3h^4(m+4k)/12} \\ &= 1 - \frac{1}{1-\frac{m^3(m+4k)h^2}{12(m^2+2km)}} \\ \frac{m^3(m+4k)h^2}{12(m^2+2km)} &= -\frac{m^3(m+4k)h^2}{12l^2} \end{aligned}$$

Now when $l = k$ then $m = 0$ and $A_h = A$. The original algorithm is less accurate at the low modes compared with high modes while the v equation is most accurate at low modes.

4 Scattering

We next consider the three dimensional scattering around some body. The two dimensional problem will be described later. Define

$$B(\theta,\varphi)v = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial v}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 v}{\partial\varphi^2} \tag{24}$$

Then the Helmholtz equation in spherical coordinates is given by

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 u}{\partial\varphi^2}+r^2k^2u=0 \qquad (25)$$

$$B_1u=\frac{\partial u}{\partial r}-\left(ik-\frac{1}{r}\right)u=O(\frac{1}{r^3}) \quad \text{as} \quad r\to\infty$$

We have expressed the Sommerfeld radiation condition in terms of the first BGT approximation [5]. Defining a new variable $s=kr$ then both the Helmholtz equation and the Sommerfeld radiation condition are independent of k in the s coordinate, i.e. k directly affects the solution only through the r variable. Another way that k can enter the solution is through the boundary condition on the scatterer for the scattered wave. So we define a new variable given by the fundamental solution (see also [19])

$$u=v\frac{e^{ikr}}{kr} \qquad (26)$$

We stress that this is based on spherical waves rather than the plane waves used for the wave guide. For general configurations one can replace the spherical distance r by an ellipsoidal or spheroidal coordinate (see e.g. [9]). Li et.al [27] consider a similar transformation without the denominator in the context of infinite elements. However, to fully account for the fundamental solution and not just the oscillatory portion it is more accurate to include the denominator $\frac{1}{kr}$ in the transformation. As an example of this change of variables consider a plane wave $u^{\text{inc}}(x)=e^{ikx\cos\theta}$ impacting on a sphere (either hard or soft) of radius a. The exact solution for the scattered wave along the z axis is given by [8, 11]

$$u=-\sum_{n=0}^{\infty}i^n(2n+1)a_nh_n^{(1)}(kr)P_n(\cos\theta) \qquad (27)$$

for a soft sphere $a_n=\dfrac{j_n(ka)}{h_n^{(1)}(ka)}$ for a hard sphere $a_n=\dfrac{j_n'(ka)}{h_n^{(1)\prime}(ka)}$

The spherical Hankel functions $j_n(kr)$ and $h_n(kr)$ both have the form

$$\frac{e^{ikr}}{kr}\sum_{m=0}^{n}\frac{b_{nm}}{(kr)^m}$$

v satisfies the equation (see (24))

$$\triangle v + 2\left(ik - \frac{1}{r}\right)\frac{\partial v}{\partial r} = \frac{\partial^2 v}{\partial r^2} + 2ik\frac{\partial v}{\partial r} + \frac{1}{r^2}B(\theta,\varphi)v = 0 \qquad (28)$$

$$\widetilde{B}_1 v = \frac{\partial v}{\partial r} = 0 \quad \text{at outer boundary}$$

For the function v we get the functional form

$$v = \frac{1}{k}\sum_{n=0}^{\infty}\frac{b_n}{(kr)^n}F_n(\theta,\varphi) \ = \frac{b_0}{k}F_0(\theta,\varphi) + ... \quad F_n \text{ independent of } k \qquad (29)$$

i.e. v has no oscillatory part that depends explicitly on k just terms that decay in r. The number of significant terms depends linearly on the wavenumber k. Hence, we hope that a numerical approximation to this problem for v should require a grid that only depends on the points per wavelength. For other bodies there might be some dependence greater than linear in k in the θ and φ directions in the near field but not the far field. Outside a sphere surrounding the scatterer one can prove [11]

$$u(x) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{nm}h_n^{(1)}(kr)Y_n^m(\hat{x})$$

converges absolutely and uniformly on compact subsets. The approximation to the equation is Hermitian when finite differences are used. The properties of a finite element approximation depends on the details of the integration formulae. Hence, for a Dirichlet condition at the scatterer the total problem for v can be Hermitian symmetric. Instead of the first BGT radiation condition we can improve this to BGT-2

$$B_2 u = \frac{\partial^2 u}{\partial r^2} + \frac{4}{r}\frac{\partial u}{\partial r} + \frac{2}{r^2}u = 0 \qquad (30)$$

$$\widetilde{B}_2 v = \frac{\partial^2 v}{\partial r^2} + \frac{2}{r}\frac{\partial v}{\partial r} = 0$$

The second derivative with respect to r is eliminated by using the differential equation. Using (28) we can rewrite this as

$$\frac{\partial v}{\partial r} = -\frac{1}{2r(1-ikr)} B(\theta, \varphi) v \tag{31}$$

This destroys the Hermitian symmetry of the matrix.

The definition of the far field pattern is

$$u(x) = \frac{e^{ikr}}{r}\left(u_\infty(\frac{x}{r}) + O\left(\frac{1}{r}\right)\right)$$

Since $v = \frac{e^{ikr}}{kr}$ this translates to

$$kv(x) = u_\infty(\frac{x}{r}) + O\left(\frac{1}{kr}\right)$$

Using (29) we can improve this to

$$kv + kr\frac{\partial v}{\partial r} = u_\infty(\frac{x}{r}) + O\left(\frac{1}{k^2 r^2}\right)$$

$$kv + kr\frac{\partial v}{\partial r} + \frac{k}{2}\frac{\partial}{\partial r}\left(r^2\frac{\partial v}{\partial r}\right) = kv + 2kr\frac{\partial v}{\partial r} + \frac{kr^2}{2}\frac{\partial^2 v}{\partial r^2} = u_\infty(\frac{x}{r}) + O\left(\frac{1}{k^3 r^3}\right)$$

4.1 Two Dimensional Scattering

In polar coordinates the Helmholtz equation is given by

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + k^2 u = 0 \tag{32}$$

and

$$u(x) = \frac{e^{ikr}}{\sqrt{r}}\left(u_\infty(\frac{x}{r}) + O\left(\frac{1}{r}\right)\right)$$

In two dimensions (26) is replaced by

$$u(r, \theta) = H_0^{(1)}(kr) v(r, \theta) \tag{33}$$

Then we have

$$\triangle v - 2k\frac{H_1^{(1)}(kr)}{H_0^{(1)}(kr)}\frac{\partial v}{\partial r} = 0 \tag{34}$$

However,

$$-2k\frac{H_1^{(1)}(kr)}{H_0^{(1)}(kr)} + \frac{1}{r} = 2ik\left[1 + \frac{1}{8k^2r^2} + O\left(\frac{1}{k^4r^4}\right)\right]$$

So we can approximate (34) as

$$\triangle v + \left(2ik - \frac{1}{r} + \frac{1}{8k^2r^2}\right)v = \frac{\partial^2 v}{\partial r^2} + 2ik\left(1 + \frac{1}{8k^2r^2}\right)\frac{\partial v}{\partial r} + \frac{1}{r^2}\frac{\partial^2 v}{\partial \theta^2} = 0$$

We will drop the $\frac{1}{8k^2r^2}$term for all the results and so solve

$$\frac{\partial^2 v}{\partial r^2} + 2ik\frac{\partial v}{\partial r} + \frac{1}{r^2}\frac{\partial^2 v}{\partial \theta^2} = 0 \tag{35}$$

In two dimensions the first two BGT far field boundary conditions are (see [5] and [29])

$$\begin{aligned} B_1 u &= \frac{\partial u}{\partial r} - \left(ik - \frac{1}{2r}\right)u = 0 \\ B_2 u &= 2\left(ik - \frac{1}{r}\right)\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + \left(2k^2 + \frac{3ik}{r} - \frac{3}{4r^2}\right)u = 0 \end{aligned} \tag{36}$$

We can approximate (33) by

$$u(r,\theta) = \frac{e^{ikr}}{\sqrt{kr}}v(r,\theta) \tag{37}$$

Then (36) becomes

$$\begin{aligned} \widetilde{B}_1 v &= \frac{\partial v}{\partial r} = 0 \\ \widetilde{B}_2 v &= 2\left(ik - \frac{1}{r}\right)\frac{\partial v}{\partial r} + \frac{1}{r^2}\frac{\partial^2 v}{\partial \theta^2} - \frac{1}{4r^2}v = 0 \end{aligned} \tag{38}$$

We can get a more accurate far field boundary condition by using an expansion in terms of Hankel functions rather than inverse powers of r. This is equivalent (through second order) with a local approximation of the DtN operator [17]. The far field generalization of (36) is

$$B_1 u = \frac{\partial u}{\partial r} - k\frac{H_0'(kr)}{H_0(kr)}u = 0 \tag{39}$$
$$B_2 u = \frac{\partial u}{\partial r} - k\left[\frac{H_0'(kr)}{H_0(kr)}u + \left(\frac{H_0'(kr)}{H_0(kr)} - \frac{H_1'(kr)}{H_1(kr)}\right)\frac{\partial^2 u}{\partial\theta^2}\right] = 0$$

where $H_0'(kr) = -H_1(kr)$ and $H_1'(kr) = 0.5(H_0(kr) - H_2(kr))$. Translating this to v defined by (33) we get

$$\widetilde{B}_1 v = \frac{\partial v}{\partial r} = 0 \tag{40}$$
$$\widetilde{B}_2 v = \frac{\partial v}{\partial r} - k\left(\frac{H_0'(kr)}{H_0(kr)} - \frac{H_1'(kr)}{H_1(kr)}\right)\frac{\partial^2 v}{\partial\theta^2} = 0$$

For three dimensions there exist similar formulae in terms of spherical Hankel functions. Thompson and Pinsky [31] and later Harari and Djellouli [22] have shown that through second order these are identical to the BGT far field boundary conditions (30).

5 Results

5.1 Waveguide

We solve (3) by a linear finite element method. This is equivalent to

$$\frac{1}{3}\left(u_{i,j+1} + u_{i,j+1} + u_{i+1,j-1} + u_{i+1,j} + u_{i+1,j+1} + u_{i-1,j-1} + u_{i-1,j}\right.$$
$$\left.+u_{i-1,j+1} - 8u_{i,j}\right) + \frac{k^2h^2}{36}\left(u_{i+1,j-1} + u_{i+1,j+1} + u_{i-1,j-1} + u_{i-1,j+1}\right.$$
$$\left. + 4u_{i,j+1} + 4u_{i,j+1} + 4u_{i+1,j} + 4u_{i-1,j} + 16u_{i,j}\right) = 0$$

The accuracy of a linear finite element method for the Helmholtz equation depends on k^3h^2. However, for the wave guide problem there is also the mode

number l, and the solution behaves as $e^{ik\sqrt{1-\frac{l^2}{k^2}}x}\sin(ly)$. It is not clear from finite element estimates how the accuracy depends on l, see however, [12]. In [21] it is shown how one can improve the accuracy by replacing the k^2h^2 that appears in the linear element algorithm by $2(1-\cos(kh))$. We shall refer to this as the stabilized method. We also solve for $v=ue^{-ikx}$ and translate back to u. We consider $0<x,y<1$ with homogeneous Neumann conditions at top and bottom, $u=\cos(l\pi y)$ at $x=0$ and a radiation condition, $\frac{\partial u}{\partial x}+iku=0$ at $x=1$. In table 1 we display the absolute L_2 error for the wave guide with various values of k,h,l.

k	$N=\frac{1}{h}$	l	pt/wave	k^3h^2	linear	stab	v
6	20	1	21	.54	.010	.005	.001
24	20	1	5	34.5	.66	.04	.00025
24	80	1	21	2.1	.050	.0027	.00001
24	80	4	21	2.1	.036	.024	.004
24	160	1	42	.54	.013	.0006	.000004
24	160	4	42	.54	.009	.006	.001
20	120	1	37	.55	.012	.0012	.0000077
20	120	4	37	.5	.009	.008	.0029
44	80	4	11.5	13.3	.269	.050	.002
80	80	4	6.3	80	1.35	.106	.001
100	10	10	6.3	100	1.44	.402	.025

Table 1: comparison of schemes for various k,h and l

Comparing $k=6$, $N=20$, $l=1$ with $k=24$, $N=160$, $l=1$ and $l=4$ we see that the error is a function of k,h and l and not just k^3h^2. This is most obvious for the stabilized method and the transformation to v variables which are exact for $l=0$ and so very accurate when $\frac{l}{k}<<1$. For l fixed and increasing k, and constant kh the error decreases! For the case where a general function $f(y)$ is given at the inlet it will depend on the Fourier expansion of f. If the Fourier components of f are band limited we expect the accuracy to increase as we increase k relative to the largest significant component in the Fourier expansion of f. However, if f has many significant modes with high l then as we increase k and N more Fourier components will become significant and the error gets larger as we increase k. For linear elements the error for $l=1$ is larger than for $l=4$ as is shown by the dispersion analysis. We see that stabilization helps but (5, 6) is by far the best.

5.2 Bands of k

We next consider predicting the solution at $u(k+\Delta k)$ as described above based on [15]. The Taylor series usually does not converge. Hence, we shall only present the Padé expansion of the Taylor series. In [15] Djellouli et. al. also consider an acceleration based on the epsilon algorithm but we found the Padé expansion to be more robust. This Padé acceleration is done at each point of the mesh independently. We compare three ways of calculating the new solution: First the Padé based on an expansion in u as presented in [15]. Second use of the recursion formula (20) and finally a Padé based directly on solving the equation (12) for v. In table 2, we show in parenthesis the order of the numerator and denominator of the Padé expansion.

Thus, using the transformation (20) improves the accuracy compared with the original method. This improvement occurs only if the mesh is fine enough so that the higher derivatives have some accuracy. A Taylor series is not useful since the higher derivatives have L^2 errors of several orders of magnitude. The acceleration procedures dramatically improve this. Nevertheless the conversion of derivatives of u to derivatives of v requires some minimal accuracy in the derivatives for the acceleration techniques to work. Thus, for $k = 24$ and $\Delta k = 20$ a mesh of 20 elements does not improve the convergence of the expansion while a mesh of 80 enables the Padé acceleration to work. Similarly for $k = 44$ and $\Delta k = 22$ a mesh of N=80 elements is not sufficient but the acceleration is useful with $N = 160$. However, solving (6) is much more accurate than both other approaches.

k	Δk	N	l	u	recursion	v
6	3	20	1	.036 (5,5)	.035 (5,5)	.010 (5,5)
24	20	20	1	1.42 (5,5)	.760 (1,1)	.0005 5,5)
24	20	80	1	1.13 (5,5)	.107 (5,5)	.0001 (5,5)
24	20	80	4	1.13 (5,5)	.254 (5,5)	.055 (5,5)
44	22	80	4	1.46 (5,5)	.630 (5,5)	.007 (5,5)
44	22	160	4	1.37 (5,5)	.312 (5,5)	.010 (5,5)

Table 2: comparison of schemes for predicting solution of waveguide at $k+\Delta k$

We next consider the more difficult case of scattering about a two dimensional submarine-like figure. This is a non-convex body and so a harder

test. The case computed is $k_0 a = 63$, $h_{k0} = \frac{a}{400}$. An unstructured mesh is used with 773,288 nodes and there is about 40 points per focal wavelength. The outer surface is situated at one wavelength from the submarine. The Helmholtz equation is solved by FETI-H. The second order BGT absorbing boundary condition is used. The Taylor series is accelerated with the ϵ algorithm (0,28) using 29 terms. The error is calculated by comparing the series expansion for $u(k_0 + \Delta k)$ with a direct Helmholtz solution at this new k. Since v is only used to find the solution at neighboring k the computer time required by the recursion formulas is negligible. See [15] for further details about the case. A sketch of the submarine is given in figure 1. We present the relative errors in table 3. Errors until about 6 % are listed. We see that the new formulation allows for a larger band of Δk to be solved within the error tolerance. The errors are not symmetric in Δk.

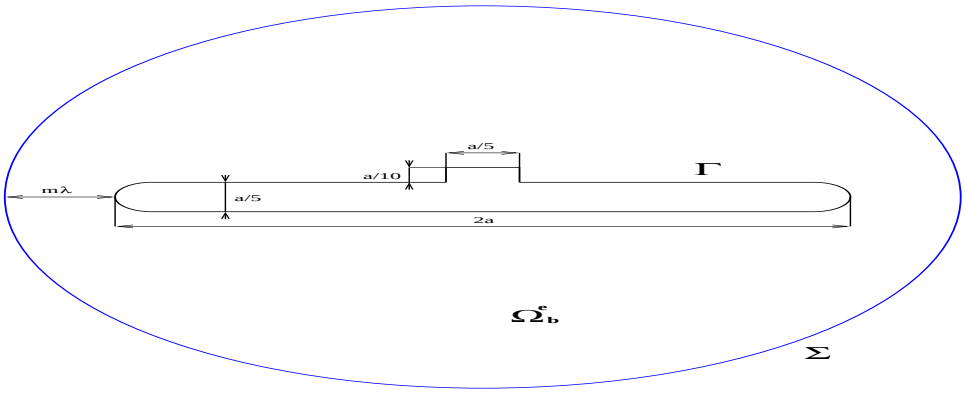

Figure 1: Submarine

5.3 Two Dimensional Scattering

For notational purposes we refer to the solution of the Helmholtz equation using linear elements as "helm". The solution of the modified equation (28) in three dimensions is denoted as "N" (nonoscillatory). In two dimensions we distinguish between "N-H" using the Hankel function, (34), and its approximation in $\frac{1}{r}$ denoted as "N-$\frac{1}{r}$". Similarly, we shall refer to the absorbing boundary condition using the Hankel function, (39), as BGTH and its approximation in $\frac{1}{r}$, (35), as BGTR. In three dimensions we only have BGT,

Δk	u	recursion	v
-9.0			.0591
-8.5			.0327
-8.0			.0219
-7.5			.0141
-7.0		.0623	.0090
-6.5		.0301	.0043
-6.0	.0518	.0179	.0020
-5.5	.0246	.0059	.0009
-5.0	.0106	.0034	.0005
-4.5	.0042	.0014	.0002
-4.0	.0010	.0004	.0000
-3.0	.0000	.0000	.0000
-2.0	.0000	.0000	.0000
-1.0	.0000	.0000	.0000
1.0	.0000	.0000	.0000
2.0	.0000	.0000	.0000
3.0	.0000	.0000	.0000
4.0	.0014	.0004	.0000
4.5	.0048	.0015	.0003
5.0	.0159	.0057	.0009
5.5	.0397	.0134	.0021
6.0	.0687	.0231	.0033
6.5		.0459	.0069
7.0			.0135
7.5			.0218
8.0			.0400
8.5			.0790

Table 3: submarine - comparison for predicting solution at $k+\Delta k$

(30). BGT-1 and BGT-2 refer to the first order and second order absorbing boundary conditions respectively.

We consider scattering around a disk of radius $R = 1$. We solve for the scattered wave and so impose a Dirichlet condition on the disk given by a plane wave. The far field boundary condition is imposed at $r = Rmax$ which is varied. We specify either BGT-1 or BGT-2 at the outer boundary. The mesh is a polar mesh with equal spacing in both r and θ. A linear element code is used to solve the equation. We compare both the absolute L^2 error and also the relative L^2 error over the domain. The exact solution is an infinite series involving Bessel functions and is given in (27).

We compare three approaches to solving the scattering problem. The first is to solve directly the Helmholtz equation (32). The second approach is to solve the equation (34) for v and then convert from v to u. The last approach is to simplify the Hankel functions that appear in (34) and then we get (35) for v. We also experiment using the Hankel function in the far field boundary equation or alternatively its expansion in $\frac{1}{r}$ as it appears in the BGT boundary condition.

In table 4, we first consider a case with $k = 3$. We choose the mesh so we have about 20 points per wave length in both r and θ. When the outer surface is very close to the inner surface there are more per wave length since the domain is so thin. We present both the L^2 volumetric error and also this error relative to the L^2 norm of the solution.

$Rmax$	BC	$\#r$	$\#\theta$	helm err-L^2	helm relerr	N-H err-L^2	N-H relerr	N-$\frac{1}{r}$ err-L^2	N-$\frac{1}{r}$ relerr
1.1	1	3	60	.032	.041	.033	.042	.033	.042
1.1	2	3	60	.005	.007	.006	.008	.006	.008
2	1	10	60	.131	.056	.126	.054	.126	.054
2	2	10	60	.020	.008	.010	.004	.011	.005
3	1	20	60	.095	.029	.073	.022	.074	.023
3	2	20	60	.043	.013	.007	.002	.007	.002
5	1	40	60	.126	.028	.034	.007	.041	.009
5	2	40	60	.115	.025	.013	.003	.014	.003

Table 4: Two dimensional scattering around disk $R=1$, $k=3$

5.3.1 Absorbing Boundary Condition

When the outer boundary is not close to the inner boundary then the use of the v equation gives a significant improvement over the original Helmholtz equation. This is especially true for the far field boundary condition BGT-2 where we have a decrease in the error by a factor of about 6-8 for $Rmax = 3$ and 5. When the outer boundary is only at $Rmax = 2$ the improvement is about two for BGT-2. This is because the series expansion for the solution is only slowly convergent near the boundary where r is not large. When the outer boundary is almost next to the inner boundary (so we almost have an on surface boundary condition) there is no improvement when using the v equation. Using the approximation for the Hankel function in the equation (i.e. (35) instead of (34)) does not seriously degrade the accuracy. Only for $Rmax = 5$ and BGT-1 is there any noticeable difference.

We also consider the effect of the replacement of the Hankel functions by their asymptotic formulae in the far field boundary condition, i.e. (36, 38) versus (39, 40). For the standard Helmholtz equation we did not see any noticeable difference. However, for (34) or (35) we found the far field boundary condition using the Hankel function more accurate at $k = 3$. When the outer boundary is very close to the inner boundary then (38) is marginally more accurate than (40). Eq. (35), in table 4 is computed using the Hankel functions in the BGT-2 boundary condition (40). We now only consider (35) with BGT-2 and compare the use of the Hankel function (40) with its asymptotic formula (38) in table 5. We conclude that for $k = 3$ the DtN formula, (39), in two dimensions has some improvement over BGT-2.

$Rmax$	$\#r$	$\#\theta$	BGT-$\frac{1}{r}$ err	BGT-$\frac{1}{r}$ relerr	BGTH err	BGTH relerr
1.1	3	60	.006	.008	.005	.007
2	10	60	.013	.011	.005	.005
3	20	60	.007	.002	.010	.004
5	40	60	.014	.003	.023	.005

Table 5: Errors in two dimensional scattering with BGT-2, k=3

We next consider in table 6 a similar computation but with $k = 5$. We only consider the second order far field boundary condition BGT-2. We choose the mesh so that we have about 25 points per wavelength in both r and θ. As before when the outer surface is very close to the scatterer there are more points per wave length.

$Rmax$	$\#r$	$\#\theta$	helm err(L^2)	helm relerr	N-H err(L^2)	N-H relerr	N-$\frac{1}{r}$ err(L^2)	N-$\frac{1}{r}$ relerr
1.1	3	128	.010	.014	.011	.015	.011	.014
1.5	10	128	.020	.012	.019	.011	.021	.013
2	20	128	.016	.007	.008	.003	.008	.004
3	40	128	.043	.013	.008	.002	.013	.004
5	80	128	.120	.027	.014	.003	.022	.005

Table 6: Two dimensional scattering around disk $R=1$, $k=5$

The general conclusions for this higher value of k are the same as before. However, now there is not much of a difference if the second order far field boundary condition is based on (38) or (40). Presumably this is because k is larger. Since we use the same domains and $Rmax$ is the same we have that $k \cdot Rmax$ is larger and so the asymptotic expansion of the Hankel functions is more accurate at the outer boundary.

We next investigate the effect of the expansion of the Hankel functions in the far field boundary condition BGT-2. For larger values of ka the differences are negligible. Consider low wavenumbers e.g. $ka = 0.01$. In table 7 we present the standard Helmholtz equation (32) with the far field boundary condition given by (36) or (39). We show both the relative L^2 error over the entire domain and the relative L^2 error of the normal derivative measured on the scatterer. The results in the table demonstrate that using (39) gives very accurate solutions independent of the position of the outer boundary. In contrast using the approximation (36) does not give reasonable solutions when measuring the error on the scatterer. The absolute L^2 error in the normal derivative on the surface behaves similarly.

$Rmax$	$\#r$	$\#\theta$	BGT-$\frac{1}{r}$ vol	BGTH vol	BGT-$\frac{1}{r}$ $\frac{\partial u}{\partial n}$ surf	BGTH $\frac{\partial u}{\partial n}$ surf
1.1	10	60	.010	.00002	.888	.0002
2	10	60	.060	.00004	.577	.006
3	20	60	.080	.00006	.432	.006
5	40	60	.095	.00007	.295	.006

Table 7: Two dimensional scattering using the Helmholtz equation, $k = 0.01$

We repeat the calculation using equations (34) and (35) for v and boundary conditions (38) and (40). To avoid area norms over different size domains

we present the L^2 error of the normal derivative of u integrated over the surface of the circle normalized by the L^2 norm of the derivative. These are presented in table 8. We find that for low wavenumbers using the Hankel function gives much more accurate results than using an expansion in $\frac{1}{r}$, (36). The effect from the boundary condition is more dramatic than the effect on the equation itself. For higher wavenumbers the approximation of the Hankel function in either the equation or the far field boundary condition does not significantly change the accuracy.

$Rmax$	$\#r$	$\#\theta$	N-H+BGT-$\frac{1}{r}$	N-H+BGTH	N-$\frac{1}{r}$+BGT-$\frac{1}{r}$	N-$\frac{1}{r}$+BGTH
1.1	10	60	.592	.00025	.558	.0015
2	10	60	.434	.0004	.292	.006
3	20	60	.351	.0004	.191	.007
5	40	60	.266	.0004	.113	.007

Table 8: Use of the Hankel function (for N) compared with $\frac{1}{r}$, $k=0.01$

We next display the L^2 error in the solution calculated on concentric circles for both Dirichlet and Neumann boundary conditions on the scatterer. We compare the solutions of the Helmholtz equation and (34) for $k=10$. The outer radius is at $r=4$. For Dirichlet boundary conditions the error is zero along the scatterer. For the Helmholtz equation the error increases linearly as r increases. However, the error is independent of r when using (34). A disadvantage of the new equation is that the error using the Helmholtz equation is slightly smaller along the scatterer. Hence, the error in calculating the far field pattern is slightly smaller using the Helmholtz equation rather than (34). We repeat the computation with only 10 elements in the radial direction. We see in figure 3 that the solution to the Helmholtz equation deteriorates rapidly when we reduce the number of elements in the r direction while the numerical approximation to (34) is still reasonable. Thus, a major benefit of the new formulation is the ability to use much coarser meshes in the r direction than are required with the Helmholtz equation.

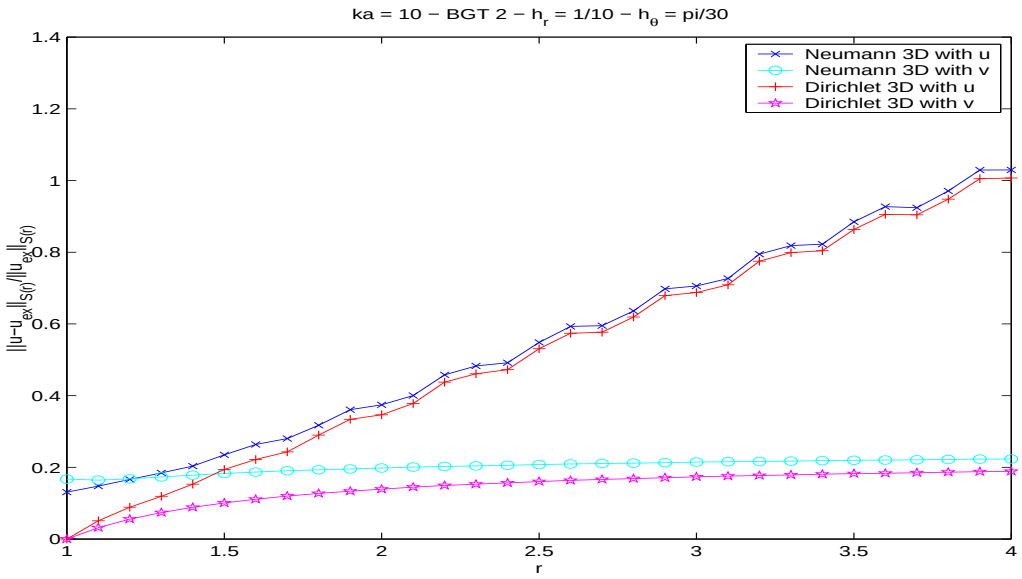

Figure 2: L^2 error of u on concentric spheres - 30 elements in r

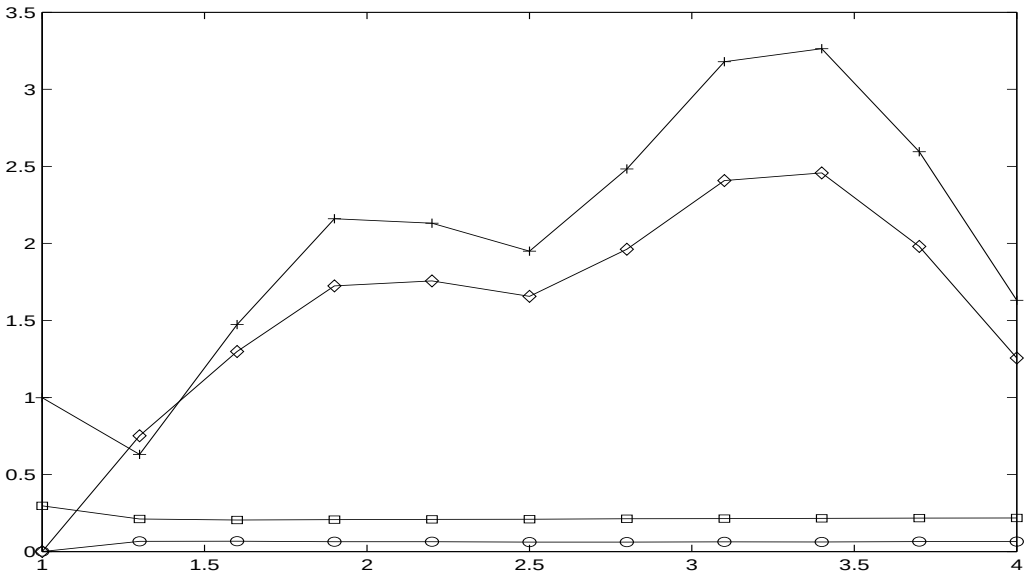

Figure 3: same as figure 2 but with 10 elements in r

5.4 Three Dimensional Scattering

We now consider scattering around a sphere. We assume that the solution is independent of ϕ and so only two independent variables appear even though the problem is three dimensional. We present the errors in table 9.

$Rmax$	BC	#r	$\#\theta$	helm err(L^2)	helm relerr	N err(L^2)	N relerr
1.1	1	3	60	.023	.054	.0236	.054
1.1	2	3	60	.005	.011	.005	.011
2	1	10	60	.086	.067	.083	.065
2	2	10	60	.010	.008	.005	.004
3	1	20	60	.058	.033	.049	.028
3	2	20	60	.021	.012	.0026	.0015
5	1	40	60	.065	.026	.026	.010
5	2	40	60	.057	.023	.003	.001

Table 9: Three dimensional scattering around sphere $R=1$, $k=3$

We have improvements of a factor of 20 when using the second order boundary condition. As before when the outer boundary is very close to the scatterer then there is not much improvement but both are very good. As previously mentioned the approximate DtN and the BGT far field boundary conditions are identical in three dimensions at least through second order.

Finally, we consider the number of elements needed to obtain a given accuracy as a function of k and h for both the Helmholtz equation and the nonoscillatory version, (34). We use the second order BGT boundary condition, (40). We fix the desired accuracy at 10% relative accuracy measured in both the L^2 norm of the area of integration and the L^2 norm of the normal derivative on the surface. We also vary the position of the outer boundary. We see, in table 10, that approximations to (28) yield more accurate solutions than those to the Helmholtz equation but the pollution still exists. A rough calculation indicates that for the original Helmholtz equation linear finite elements requires about $N_\theta = 1.56k^{\frac{3}{2}}$ points while the new formulation requires about $N_\theta = 1.33k^{\frac{3}{2}}$ points. It is interesting that the new formulation requires fewer points in the θ direction even though the transformation is only in the r direction. The original Helmholtz formulation also requires that N_r increases with $k^{\frac{3}{2}}$ while the new formulation requires N_r to increase

faster than linear in k but less than $k^{\frac{3}{2}}$. Also, for fixed k the Helmholtz formulation requires the number of points in r to increase faster than linear as we move the artificial boundary further out. However, (26) requires only a linear growth in the number of points in the r direction as a function of r. This is because the error does not grow in r for the new formulation while it does grow for approximations to the Helmholtz equation (see figures 2 and 3). The number of points required in each direction is difficult to calculate since one can trade off points in r against the number of points needed in θ to achieve a given accuracy.

We further see that the position of the outer boundary can be approximately independent of k. For low values of ka the outer boundary can be brought quite close to the scatterer. In fact on-surface boundary conditions work well [25]. For larger values, e.g. $ka \geq 40$ accurate solutions could not be obtained if the outer surface is too close to the scatterer. This is in contrast to [29] and [14] that chose $Rmax = R_0 + \frac{\text{const}}{k}$. That choice implies that for the Laplace equation one needs the outer boundary far from the scatterer while for large k the outer boundary can be extremely close to the scatterer. The computations performed here do not agree with these conclusions. The poor behavior of the BGT boundary condition for large k in [29] is due to the positioning of the outer boundary too close to the scatterer rather than any intrinsic difficulties with the local BGT boundary conditions. For the simple problems presented here one can choose the outer boundary close to the scatterer. For more complex geometric shapes this may no longer be true. Hence, the error as a function of the distance of the outer boundary is of importance.

The code is written in MATLAB and uses an internal linear equation solver based on the symmetric reverse Cuthill-McKee ordering. CPU times for solving the Helmholtz and preconditioned "v" formulations depend on the details of the linear solver. Choosing $k=40$, $Rmax=2$ and using a mesh 40×340, solving for u required 35.2 seconds while solving for v required 51.1 seconds (using a Pentium 4 2Ghz processor under MS windows). The extra time is due to the loss of the symmetric complex form. For equal accuracy the Helmholtz equation needs a mesh of 115×400 which required 186 seconds which is more than three times as expensive as solving as solving the preconditioned equation with the loss of symmetry.

k	$k^{\frac{3}{2}}$	scheme	$Rmax$	$\#r$	$\#\ \theta$	#tot	vol	$\frac{\partial u}{\partial n}$	FPP
5	11	u	1.1	3	18	76	.012	.053	.060
		u	2	8	18	171	.056	.077	.088
		u	3	18	18	361	.092	.086	.080
		u	4	35	18	684	.096	.054	.084
		v	1.1	3	16	68	.011	.050	.048
		v	2	4	15	80	.040	.091	.060
		v	3	8	15	144	.048	.091	.061
		v	4	12	15	208	.055	.091	.062
10	32	u	1.1	3	50	204	.031	.069	.032
		u	2	16	50	867	.082	.094	.058
		u	3	48	50	2499	.099	.045	.053
		u	4	100	50	5151	.099	.029	.052
		v	1.1	3	40	164	.090	.077	.048
		v	2	8	40	369	.048	.100	.085
		v	3	16	40	697	.061	.095	.084
		v	4	24	40	1025	.070	.094	.084
20	89	u	1.1	3	140	564	.067	.099	.086
		u	2	40	140	5781	.094	.070	.029
		u	3	140	140	19881	.098	.021	.031
		u	4	290	140	41031	.100	.015	.030
		v	1.1	5	115	596	.067	.097	.089
		v	2	18	115	2204	.060	.094	.093
		v	3	36	115	4292	.076	.091	.090
		v	4	54	115	6380	.085	.091	.091
40	256	u	1.1	15	400	15708	.100*	.067	.065
		u	2	115	400	46516	.096	.032	.020
		u	3	390	400	156791	.099	.012	.018
		u	4	815	400	327216	.100	.009	.017
		v	1.1	15	340	5456	.104*	.075	.064
		v	2	40	340	13981	.078	.096	.093
		v	3	80	340	27621	.093	.094	.094
		v	4	125	340	42966	.100	.088	.087

Table 10: Relative error for three dimensional scattering around sphere
$*$ adding nodal points doesn't improve accuracy. Accuracy limited by closeness of outer boundary.

6 Parabolized Equation

In spherical coordinates v satisfies the equation (see (24))

$$\frac{\partial^2 v}{\partial r^2} + 2ik\frac{\partial v}{\partial r} + \frac{1}{r^2}B(\theta,\varphi)v = 0$$

When v is a smooth function in r we assume that the second derivative v_{rr} is small compared with the first derivative $2ikv_r$. Dropping the second derivative term we get

$$\frac{\partial v}{\partial r} = -\frac{1}{2ikr^2}B(\theta,\varphi)v \tag{41}$$

This is a parabolic equation that can be marched in r instead of an elliptic equation which requires the inversion of a matrix. Marching from the body outwards we no longer need a boundary condition at $r = \infty$. This three dimensional equation is appropriate for scattering problems. It is the direct analog of the parabolic equations of Claerbout [10] and Tappert [30] in two dimensional Cartesian and cylindrical coordinates for problems in seismology and underwater acoustics.

Using the expansion (29) $v_{rr} = -\frac{2}{r}v_r + O(\frac{1}{kr})$. Instead of eliminating the second derivative we can, to higher order, replace it by a first derivative. Hence, to higher order in $\frac{1}{kr}$, we replace (41) by

$$\frac{\partial v}{\partial r} = \frac{1}{2r(1-ikr)}B(\theta,\varphi)v = \frac{ikr+1}{2(1+k^2r^2)r}B(\theta,\varphi)v \tag{42}$$

This is an extension of the parabolic approximations and is also a parabolic equation similar to (41). This is higher order accurate in $\frac{1}{kr}$ and not higher in the angle as is usually done, see for example [10, 24]. This equation is identical to the far field boundary condition (31). It is no longer similar to the Schroedinger equation because the coefficient on the right hand side is not pure imaginary. However, a trapezoidal (Crank-Nicolson) scheme still leads to unconditional stability. Though the scheme is implicit this leads to a system of equations in the other variables besides r while the Helmholtz equation requires the inversion of a matrix in all three variables.

Another way of looking at the same phenomena is that the parabolic equation is equivalent to a far field BGT boundary condition. Hence, for the scattering problem using a parabolic equation is equivalent to applying the

BGT boundary condition on the surface of the scatterer. Such on surface conditions (OSRC) have been considered by [25] and [1, 2]. This does not necessarily yield accurate results because the BGT boundary conditions assume r is large. The results are accurate for large wavenumbers. One can consider the parabolized equation as an extension of the OSRC. Instead of applying the far field boundary condition on the surface we march it as a parabolic equation into the far field.

We now consider axisymmetric cylindrical coordinates. Similar to the two dimensional wave guide we consider a substitution

$$u(r,z) = v(r,z)H_0^{(1)}(k_0 r)$$

Using the asymptotics of the Hankel function we get (see (35))

$$v_{rr} + 2ik_0\left(1 + \frac{1}{8k_0^2r^2}\right)v_r + v_{zz} = 0 \tag{43}$$

Assuming that the variation in r is small then v_{rr} is small compared with v_r. Dropping the v_{rr} and $\frac{1}{8k^2r^2}$ terms (43) is replaced by

$$2ik_0 v_r + v_{zz} = 0 \tag{44}$$

This is a parabolic equation was used by Tappert [30] for problems in underwater acoustics while Claerbout [10] applied it to seismology. Instead of eliminating v_{rr} we can replace it by its asymptotic expansion $v_{rr} \sim -\frac{2}{r}v_r$. Then (44) is replaced by

$$2\left(ik_0 - \frac{1}{r}\right)v_r + v_{zz} = 0 \tag{45}$$

The improvement to account for additional terms in the $\frac{1}{kr}$ expansion can also be made to the higher order (in angle) parabolic approximations.

Djellouli et. al. introduced [15] a series expansion in k to find $u(k+\Delta k)$ for the Helmholtz equation. One can do the same for the parabolic equation. The application is easier since there is no boundary condition at the exit. Hence, k appears only in the differential equation. Labeling $v_n = \frac{1}{n!}\frac{\partial^n v}{\partial k^n}$ at k_0 from (45) we get the equation for the n-th derivative

$$2\left(ik_0 - \frac{1}{r}\right)\frac{\partial v_n}{\partial r} + \frac{\partial^2 v_n}{\partial z^2} = -2i\frac{\partial v_{n-1}}{\partial r} \tag{46}$$

7 Conclusion

We have introduced a new variable for the Helmholtz equation based on the principle of removing the main oscillatory term. This term is connected with the fundamental solution for that domain. Hence, it depends both on the geometry and the number of dimensions. Equivalently, the new variable v satisfies the first term in a separation of variables. Hence, we get a new equation that removes the main oscillatory terms for waveguide and scattering geometries in both two and three dimensions. One can also generalize the cylindrical/spherical coordinate r to spheroidal or ellipsoidal coordinates. This is the first step in the parabolic approximation [30, 10, 24]. However, in the present approach we do not make any approximations and so backscattering is fully accounted for. The same change of variables is also the first stage of the infinite element algorithm [16, 23, 29]. One expects approximations to this new variable to give accurate results for all low modes. In particular it has the property that, for a waveguide, if the boundary mode is fixed and the wavenumber, k, increases then the approximation becomes more accurate in spite of the fact that k increases. This occurs since the important parameter is the ratio of the mode number to the wavenumber. In contrast the standard finite difference and linear finite element algorithms are less accurate for low modes than for higher modes. The definition of the new variable is based on both the differential equation and the Sommerfeld radiation condition. Hence, it is expected to be accurate for outgoing waves but less accurate for any backscattered waves.

All the numerical results use a finite element code based on linear elements. Computational results are presented for a Cartesian waveguide and scattering about a circle and sphere with comparisons to the exact solution. Results have also been obtained for a non-convex two dimensional body that models a submarine. In all cases the results obtained confirmed the improved accuracy when the new equation for v is solved compared with the standard Helmholtz equation. For fine enough meshes discretizations to the Helmholtz equation and the new equation give similar results since they are analytically equivalent. The main advantage of the new approach is that it allows much coarser meshes in the radial direction and a slightly coarser mesh in θ to get comparable accuracy. One disadvantage of the new approach is that even complex symmetry is lost.

We measure the L^2 error along concentric circles around the scatterer. For the finite element approximation to the Helmholtz equation this error

grows as we go away from the scatterer. However, for (26) the line L^2 error is essentially independent of r. Thus, the volume L^2 error is much smaller for the new approach compared with the direct solution of the Helmholtz equation. The L^2 error along the scatterer is comparable in both approaches.

In addition to solving the equation for a fixed wavenumber k we also examined the possibility of finding the solution at neighboring wavenumbers based on a Taylor Series expansion accelerated by a Padé expansion (see [15]). We present several ways of implementing the new variable. The most accurate way is to directly solve for the new variable and its derivatives and calculate $v(k+\Delta k)$ and then return to $u(k+\Delta k)$. Another alternative is solve the original Helmholtz equation for u and its derivatives and then convert these to v and its derivatives. This is less accurate but requires no new coding for numerical solutions to differential equations. A last possibility is to derive a new formula for approximations to the Helmholtz equation by translating the finite element algorithm for the new variable v back to the original variable u. This new formula for u has the nice properties of the v approximation.

The fundamental solution to the two dimensional Helmholtz equation involves the Hankel function $H_0^{(1)}(kr)$. Hence, this appears in the equation for the variable v. Since, we are interested in large r we can replace this by an expansion in $\frac{1}{r}$ keeping only the first term. Because we are interested in exterior domains one needs to approximate the Sommerfeld radiation condition by a boundary condition on a finite surface. We consider the BGT absorbing boundary condition [5, 17] that is based on matching the series expansion of the solution. Again, in two dimensions this involves the Hankel function but one can replace this by its expansion in $\frac{1}{r}$. We compare the use of the Hankel function to its expansion both in the differential equation for v and in the far field boundary condition both for the Helmholtz equation and for v. Not surprisingly, we find that for moderate and large kr the differences between the two formulations is small. However, for $kr << 1$ the Hankel function formulation gives much better results even when used in the BGT boundary conditions for the Helmholtz equation. For $ka = 0.01$ there is several orders of magnitude difference in the error. In three dimensions the approximation to DtN and the BGT boundary conditions are identical [22].

We investigated the position of the outer artificial boundary, for a cylinder and sphere, as a function of k. For these simple geometries one could bring in the outer boundary quite closer to the scatterer independent of k. For larger $ka > 40$ one could not bring the outer boundary too close to the scatterer

without limiting the accuracy. In any case one would not want to choose the position of the outer boundary so that there is a fixed number of wavelengths from the scatterer. This implies that the position of the artificial boundary is inversely proportional to k. This would require too large domain for small k and conversely would bring the outer boundary too close for larger k which would limit the accuracy. This would then falsely reduce the accuracy for large k compared with infinite elements [29].

We analyze the connection of the elliptic equation obtained for the new variable v with the parabolic approximation used in underwater acoustics and seismology, [30, 10, 24]. The parabolic equation has the advantage that it can be marched and hence is computationally faster than solving an elliptic equation. On the other hand the parabolic equation completely eliminates all backscattering and has other simplifications. Hence, we expect the full elliptic equation to be more accurate especially for scattering around non-convex bodies. Similar observations pertain to the on-surface radiation conditions of [25, 1, 2]. One possibility is that either the parabolic equation or on-surface condition can be used as a preconditioner for the elliptic equation for v. One can use the parabolic equation as part of an iterative method to solve the elliptic equation for v since it is an approximation to the v equation.

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