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On Accuracy Conditions for the Numerical Computation of Waves

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The Helmholtz equation $(\Delta + K^2n^2)u = f$ with a variable index of refraction n and a suitable radiation condition at infinity serves as a model for a wide variety of wave propagation problems. Such problems can be solved numerically by first truncating the given unbounded domain, imposing a suitable outgoing radiation condition on an artificial boundary and then solving the resulting problem on the bounded domain by direct discretization (for example, using a finite element method). In practical applications, the mesh size h and the wave number K are not independent but are constrained by the accuracy of the desired computation. It will be shown that the number of points per wavelength, measured by $(Kh)^{-1}$, is not sufficient to determine the accuracy of a given discretization. For example, the quantity K^3h^2 is shown to determine the accuracy in the L^2 norm for a second-order discretization method applied to several propagation models.

INTRODUCTION

The Helmholtz equation

$$\Delta u + K^2n^2u = 0, \tag{1.1}$$

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where K is the wave number and $n(x)$ is the index of refraction, describes a wide variety of wave propagation phenomena through an inhomogeneous medium. Inhomogeneities are represented by spatial variations in $n(x)$ and also by interfaces and scattering surfaces. Equation (1.1) is fundamental in acoustics, in particular, in underwater acoustics [7, 8], duct acoustics [2, 10, 12], and acoustical scattering [5]. In addition, certain models of electromagnetic and elastic wave propagation can be described by (1.1) [11, 12]. Vector formulations of (1.1) describe general electromagnetic and elastic wave propagation [15]. Finally, the propagation of pulse-like waves can be reduced to an analysis of (1.1) after Fourier transforming the time variable [1].

If the wave length λ $(=2\pi/K)$ is small relative to the other length scales in the problem, solutions to (1.1) can be approximated by asymptotic methods. However, if λ is of the same order as some characteristic length scale, these expansions can break down and the problem must be, in general, solved by numerical methods. The methods we are considering are based on truncating the domain in which the wave propagation is occurring and imposing a suitable outgoing radiation condition on an artificial boundary. The resulting problem is then solved on the bounded domain by directly discretizing (1.1). Such a method is described in [4], where an efficient technique to solve the resulting linear system of equations is also introduced.

In general, radiation conditions do not completely absorb all reflections. The total error in the numerical solution of (1.1) is the sum of two errors: the error due to the approximate radiation condition and the discretization error due to the approximation of the continuous problem by a discrete problem. In this paper we will analyze only the discretization errors due to a standard finite element approximation scheme for (1.1), on a bounded domain with a suitable radiation condition.

In any wave propagation problem there are at least three important and distinct length scales. These are l, the diameter of the truncated computational region; a, the diameter of the region containing the inhomogeneities or other effects which distort free space wave propagation; and h, the mesh size. Since K has units $(\text{length})^{-1}$, this gives three nondimensional quantities Ka, Kl, and Kh which relate these characteristic lengths to the wavelength.

$(Kh)^{-1}$ is the number of grid points per wavelength (up to a constant factor) and has been used as a measure of accuracy by many authors (see, for example, [2, 7, 13] and the references contained therein). Ka is essentially the number of wavelengths in the inhomogeneous region and is a measure of the degree of distortion of the solution from free space wave propagation. Kl is a measure of the number of wavelengths in the computational domain. It depends on the effectiveness of the radiation boundary condition in simulating outgoing radiation and on the positions at which the solution is desired. In general, the computational domain is fixed and includes all the inhomogeneties. The wave number then varies over some range of physical interest.

In this paper it will be established that Kh is not a sufficient indicator of the truncation error of a discrete approximation to (1.1). The arguments, in general, will be given in the context of a finite element discretization, nevertheless we expect that similar results are valid for finite difference approximations. It will be shown that the discretization error depends on both Kl and Kh. Thus, when the computational domain is fixed, discretization errors will grow as K increases even though the number of points per wavelength remains fixed. If a finite element method accurate to order m is used, an error bound of $O(K^m h^{m-1})$ will be established for errors in the H^1-norm. Furthermore, an error bound of

$$O(K^{m+1+\alpha} h^m) \tag{1.2}$$

will be established for errors in the L^2-norm, where $\alpha \geqslant 0$ depends on both the geometry of the problem and the radiation condition. This estimate is suboptimal in the sense of approximation theory for the finite element subspace. We stress that this analysis is only for the discretization error and does not include the errors due to the approximation of the radiation condition at a finite boundary.

Estimate (1.2), with $\alpha = 0$, was used in [6] in discussing the usefulness of the multigrid method to solve the Helmholtz equation. In Section 2, (1.2) will be established rigorously in a fairly general setting. It will be shown that $\alpha = 0$ is the most favorable bound and is sharp for a one-dimensional model problem but that in general $\alpha > 0$. The results are obtained from a standard finite element error analysis combined with some nonstandard lemmas bounding the solution in term of the data and K. A reader only interested in the consequences of the theory can skip Section 2 and just read the precise statement of Theorem 2.2. Numerical results will be presented in Section 3 validating the theory in a waveguide geometry. In Section 4 several practical consequences of this theory will be discussed.

2. Error Estimates

We now outline the theoretical results. We first consider the model problem

$$[-\Delta - (K^2 + i\delta K)]\, u(x) = f(x), \qquad x \in \Omega, \tag{2.1a}$$

$$\frac{\partial u}{\partial n} = 0, \qquad \text{on } \partial\Omega, \tag{2.1b}$$

where $\delta > 0$, $K > 0$, Ω is a bounded domain in R^N ($N = 1, 2, 3$) with a smooth boundary $\partial\Omega$, and $f(x)$ smooth.

Remark 2.1. The term $i\delta K$ is introduced so that (2.1) is a well-posed boundary value problem. In practical problems this is accomplished by the radiation boundary condition.

To approximate (2.1) we use a finite element method and introduce a variational formulation. Let

$$a(u, v) = \int_{\Omega} [\nabla u \cdot \nabla \bar{v} - (K^2 + i\delta K)\, u(x)\, \bar{v}(x)]\, dx$$

and

$$(f, v) = \int_{\Omega} f(x)\, \overline{v(x)}\, dx,$$

then the weak form of (2.1) is

$$a(u, v) = (f, v) \qquad \text{all } v \in H^1(\Omega), \tag{2.2}$$

where $H^1(\Omega)$ denotes the standard Sobolev space. Given a subspace $S^h \subset H^1(\Omega)$ the finite element approximation is the function $u^h \in S^h$ such that

$$a(u^h, v^h) = (f, v^h) \qquad \text{for all } v^h \in S^h. \tag{2.2$'$}$$

We assume that L^2 functions can be approximated to order h^m by elements of S^h. We can then prove the following theorem.

THEOREM 2.1. *Suppose that u satisfies* (2.2) *and $u \in H^m(\Omega)$. Then there exists a unique solution u^h of* (2.2′) *provided $K^2 h$ is sufficiently small. Furthermore, the following estimates hold for the error $e^h = u - u^h$,*

$$\|e^h\|_{H^1} \leqslant C_m h^{m-1}(1 + K^m)[\|u\|_{L^2} + \gamma_m(f)], \tag{2.3a}$$

$$\|e^h\|_{L^2} \leqslant C_m h^m(1 + K^{m+1})[\|u\|_{L^2} + \gamma_m(f)], \tag{2.3b}$$

where C_m depends on m and Ω but is independent of K and the data f, γ_m is given by

$$\gamma_m(f) = \begin{cases} \dfrac{\|f\|_{L^2}}{K^2+1} + \displaystyle\sum_{j=4}^{m} \dfrac{\|f\|_{H^{j-2}}}{K^j+1}, & m \text{ even}, \quad (2.4a) \\[2ex] \dfrac{\|f\|_{L^2}}{K+1} + \displaystyle\sum_{j=3}^{m}{}' \dfrac{\|f\|_{H^{j-2}}}{K^j+1}, & m \text{ odd}. \quad (2.4b) \end{cases}$$

The sum in (2.4a) ranges over even indices while the sum in (2.4b) ranges over odd indices.

The estimate (2.3b) shows that the L^2 error (normalized by $\|u\| + \gamma_m(f)$) for a scheme of order m grows at least as fast as $h^m K^{m+1}$. We shall later show that in some cases this rate of growth is sharp. For certain classes of data f we can also show that $\gamma_m(f) \leqslant C_m \|u\|_{L^2}$, where C_m is independent of K and f. In these cases we have the estimate

$$\|e^h\|_{L^2} \leqslant C_m(1 + K^{m+1})\, h^m \|u\|_{L^2} \tag{2.5}$$

and so we have bound on the relative error $\|e^h\|_{L^2}/\|u\|_{L^2}$. An example of such a class is data f which can be expanded in a sufficiently rapidly convergent series of eigenfunctions of $-\Delta$ in Ω.

A proof of Theorem 2.1 for the model problem (2.1) will be presented elsewhere. The proof depends on the finite element analysis of [16] together with elliptic estimates and the following bound of the solution in terms of the data

$$\|u\|_{L^2(\Omega)} \leqslant \frac{C}{K} \|f\|_{L^2}, \tag{2.6}$$

where C is independent of K and f. For more general problems, (2.1b) is replaced by a radiation condition (which can be local or nonlocal, see, e.g., [3, 8–12]). The finite element analysis in [16] has been extended to problems with different radiation conditions [9, 10]. However, (2.6) is not true, in general, and the strongest bound that we can establish is

$$\|u\|_{L^2(\Omega)} \leqslant \frac{C}{K^{1-\alpha}} \|f\|_{L^2(\Omega)}, \tag{2.7}$$

where $\alpha \geqslant 0$ depends on the geometry, the dimension of the problem and the radiation condition. In such cases we can establish the following bound for the error e^h:

$$\|e^h\|_{L^2(\Omega)} \leqslant C_m(K^{m+1+\alpha}+1)\, h^m(\|u\|_{L^2(\Omega)} + \gamma_m(f)). \tag{2.8}$$

A proof of these results will appear elsewhere. We next consider the validity of (2.7) for various problems with radiation boundary conditions. It can be shown that for the one-dimensional problem

$$\begin{aligned} -\frac{d^2u}{dx^2} - K^2u(x) = f(x), \qquad & 0 \leqslant x \leqslant 1 \\ u(0) = 0, \qquad & \frac{\partial u}{\partial x}(1) = iku(1), \end{aligned} \tag{2.9}$$

where $f(x)$ vanishes near $x = 1$, (2.7) holds with $\alpha = 0$.

We next consider the Helmholtz equation in a Cartesian waveguide. Let $\Omega = \{x \in [0, \pi],\ y \in [0, \pi]\}$, and let $f = 0$ near $x = \pi$, and consider the problem

$$\begin{gathered} (-\Delta - K^2)\, u(x, y) = f(x, y), \qquad (x, y) \in \Omega, \\ u(0, y) = 0, \qquad u(x, \pi) = 0, \qquad u_y(x, 0) = 0, \quad u_x(\pi, y) = T(u), \end{gathered} \tag{2.10}$$

where $T(u)$ is the global boundary operator for outgoing modes introduced in [8, 10]. In subdomains where $f = 0$, the solution to (2.9) can be expressed as a sum of modes

$$u = \sum_{j=0}^{\infty} A_j q_j(y)\, e^{i\sigma_j x}, \tag{2.11}$$

where

$$q_j(y) = \cos((j+\tfrac{1}{2})\,y),$$
$$\sigma_j = \sqrt{K^2 - (j+\tfrac{1}{2})^2}.$$

For $K^2 - (j+\frac{1}{2})^2 > 0$, the jth mode is propagating and outgoing. For $K^2 - (j+\frac{1}{2})^2 < 0$, the jth mode decays exponentially and is called evanescent. The values $\{j+\frac{1}{2}\}$ are called cutoff frequencies. When K equals a cutoff frequency the problem is not well posed.

We can show that (2.7) holds for (2.10) with $\alpha = \frac{1}{2}$ provided K is uniformly bounded away from a cutoff frequency. Furthermore (2.7) holds with $\alpha = 0$ when the solution consists of a finite number of modes. Numerical results for a problem similar to (2.10) will be presented in Section 3. Extensions of these results to exterior problems will appear elsewhere.

For $m = 2$, the L^2 estimate with $\alpha = 0$ shows that as K increases, the L^2 error grows at a rate $O(K^3h^2)$. To show that this growth rate is sharp we consider the difference equation in one dimension

$$u_{j+1} - 2u_j + u_{j-1} + K^2h^2u_j = 0, \tag{2.12}$$

as a second-order approximation to the equation

$$u_{xx} + K^2u = 0. \tag{2.13}$$

Equation (2.12) corresponds to discretizing (2.13) with piecewise linear elements and lumping the mass matrix (i.e., the terms involving K^2 in the bilinear form). It can be seen that the argument below is also valid without lumping.

Solutions to (2.12) are of the form

$$u_j = e^{izjh} = e^{izx_j}; \qquad x_j = jh,$$

where

$$zh = \pm Kh[1 + O((Kh)^2)]. \tag{2.14}$$

If we wish to approximate the outgoing solution (as $x \to +\infty$), the $(+)$ sign must be chosen in (2.14) and the approximate solution is

$$u_j = e^{izjh} = e^{iKx_j(1 + O((Kh)^2))}.$$

Therefore, the error e_j is

$$e_j = e^{iKx_j}[e^{ix_jO(K^3h^2)} - 1],$$

and if we consider a fixed region in x and assume K^3h^2 small, we obtain

$$\|e_j\|_{L^2} / \|u\|_{L^2} = O(K^3h^2).$$

3. Numerical Results

To numerically validate the theory presented in Section 2, we consider a model problem

$$u_{xx} + u_{yy} + K^2 u = 0, \qquad 0 \leqslant x \leqslant \pi, 0 \leqslant y \leqslant \pi, \tag{3.1}$$

with boundary conditions

$$u_y(x, 0) = u(x, \pi) = 0,$$
$$u_x(0, y) = f(y),$$
$$u_x(\pi, y) = T(u),$$

where the boundary operator T will be described below. We consider three examples. In example 1, $f(y)$ is chosen so that the exact solution is

$$u(x, y) = e^{i\sqrt{K^2 - 0.25}x} \cos \frac{y}{2},$$

and $T(u) = i\sqrt{K^2 - 0.25}\, u$. In examples 2 and 3, f is chosen so that the exact solution is

$$u = \sum_{j=0}^{M} e^{il_j x} \cos((j + \tfrac{1}{2})\, y); \qquad l_j = \sqrt{K^2 - (j + \tfrac{1}{2})^2},$$

where $M = 4$ for example 2 and $M = 7$ for example 3. The boundary operator is the global operator $T(u)$ referred to earlier which was introduced in [8] for an underwater acoustics propagation model. When l_j is real, the j^{th} mode in the solution has no decay in x and is called a propagating mode. When l_j is imaginary, the jth mode decays in x and is called evanescent.

A square $N \times N$ grid is used and the equations are solved by the preconditioned conjugate gradient method described in [4]. Piecewise linear elements with lumping are used. Normalized L_2 errors for the examples are shown in Table I–III for different values of K and N.

TABLE I

Results for Example 1

K	N	Error	Kh	K^3h^2
4.16	65	0.0120	0.204	0.173
5.45	97	0.0137	0.178	0.173
6.60	129	0.0147	0.162	0.173
6.24	97	0.0182	0.204	0.260
8.32	129	0.0252	0.204	0.347

TABLE II

Results for Example 2

K	N	Error	Kh	K^3h^2
4.16	65	0.0133	0.204	0.173
5.45	97	0.0120	0.178	0.173
6.60	129	0.0114	0.162	0.173
6.24	97	0.0165	0.204	0.260
8.32	129	0.0227	0.204	0.347

In Tables I and II the first three entries correspond to K^3h^2 fixed while the first and last two entries correspond to Kh fixed. It is clear from the tables that the errors grow almost linearly in K for Kh fixed and are nearly constant for K^3h^2 fixed. In these examples, K is uniformly bounded away from the cutoff frequencies and the estimate (2.5) is confirmed numerically. (We have observed that this scaling of the error does break down as K and N are decreased. This is to be expected from the estimate (2.5) as K approaches 0.)

In Table III the first two entries correspond to K^3h^2 fixed and the first, third, and fourth entries correspond to Kh fixed. For these entries, K is not close to a cutoff frequency and the estimate (2.5) is again confirmed. The last three entries contain values of K very near a cutoff frequency. In these cases the errors do not scale as predicted and are in fact considerably worse. This is because the constant depends on how close K is to a cutoff frequency. The errors that would be observed in practice depend on the sequence of K values, how close they are to cutoff frequencies, and whether the modes close to cutoff are propagating or evanescent.

4. Implications

We conclude this paper by listing several computational implications of the results in Section 2.

TABLE III

Results for Example 3

K	N	Error	Kh	K^3h^2
4.16	65	0.013	0.204	0.173
6.24	119	0.013	0.166	0.172
6.24	97	0.019	0.204	0.260
8.32	129	0.025	0.204	0.347
5.45	97	0.029	0.178	0.173
5.55	97	0.045	0.181	0.183
6.60	129	0.036	0.162	0.173

(a) Accuracy evaluations will have to account for the number of wavelengths in the computational domain. The number of points per wavelength will have to increase with the number of wavelengths to maintain accuracy. Thus, the effects of this theory would be expected to become more important as new numerical techniques and computer technology make the numerical solution to (1.1) feasible for a larger number of wavelengths. For the simple model problem (3.1) numerical experiments with a second-order finite difference code indicate that we wish to choose the number of points N in each direction to be $N = 0.8(Kl)^{3/2}$ to achieve approximately a 7% L^2 accuracy.

(b) The precise relationship between K and h to maintain a fixed accuracy depends on both the order of the discretization scheme, the norm in which it is necessary to maintain the accuracy, and also possibly on the geometry and the boundary conditions. The advantages of using higher order methods are greater as the number of wavelengths increases.

(c) Iterative methods for the solution of the linear systems of equations obtained by discretizing (1.1) are usually analyzed by studying the convergence rate for fixed K as $h \to 0$. In practice, K and h are constrained by a given accuracy requirement and K increases over some interval. Thus, for a second-order method and accuracy determined by the L_2 norm of the error, these methods should be analyzed for K^3h^2 fixed (provided (2.5) is valid) and K increasing for the propagation models discussed in this paper.

Note added in proof. We have observed numerically a growth rate of the form (1.2) with $\alpha = \frac{1}{2}$ for a Cartesian wave guide. Thus this estimate is sharp.

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