A new algorithm for solving the wide angle wave equation

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Research Report YALEU/DCS/RR-485
September 1986

This work was supported in part by the Office of Naval Research under contracts N00014-82-K-0184, N00014-85-WR-24068, N00014-85-WR-24268, N00014-86-WR-2433, and in part by Naval Underwater Systems Center Independent Research project A65020.

Abstract. Existing techniques for solving the wide angle wave equation are traditionally obtained via a formal approximation of a square-root of a partial differential operator. Then the classical parabolic approximation implicitly consists of further replacing the resulting equation by a Pade approximation. The new approach proposed in this paper approximates the original exponential of the square-root operator directly thus avoiding the second step. Furthermore, we impose a stability condition on the aproximation so that the resulting rational function is always of modulus one. The resulting approximation is so accurate that a simple (1,1) rational approximation yields a powerful wide angle capability. The most attractive feature of the new method is that for the (1,1) approximation, the numerical finite difference technique requires that we solve only one tridiagonal system at each step. Moreover, a (2,2) rational approximation, which delivers a higher accuracy, can also be derived; in this case the numerical finite difference technique requires that we solve either two successive tridiagonal systems or, equivalently, a (narrow) pentadiagonal system. Two numerical examples are exhibited to show the wide angle capability of the new method using the (1,1) and the (2,2) rational approximations respectively.

1. Introduction

Numerical methods for solving the one-way wave equation with wide angle propagation were first introduced by Claerbout [3] who used a first order rational function approximation to a square-root operator. Following Claerbout, a number of contributions have been made in this area, especially in recent years. All of these contributions deal with the treatment of the square-root operator. Notable ones include the following: Estes and Fain [4] introduced a three-term Taylor expansion, and Berkhout [1] used a continued fraction approximation; Trefethen [12] proposed a number of different types of best approximations and least squares approximation; Greene [5] introduced a set of coefficients to improve Claerbout's approximations; Thomson and Chapman [11] applied the split-step Fourier algorithm. More recently, St. Mary and Lee [9] introduced a high order rational approximation. Concerning software, a code developed by Botseas, Lee, and Gilbert [2, 6] is frequently used. The approximations developed by Trefethen and St Mary and Lee are the most general so far.

This paper has been motivated by the fact that most contributions in this area consist of two steps. First a formal approximation of the square-root of a partial diffierential operator is obtained. Then to derive a one-step integration scheme with respect to range, the so-called parabolic approximation implicitly consists of using a further approximation, usually of the Pade type, to approximate the exponential operator. Our new approach approximates the original exponential of the square-root operator directly, thus avoiding the second step. The result will be a much more accurate approximation in general. Stability of the derived scheme is *guaranteed* by imposing that the numerator and the denominator of the rational approximation be conjugate of each other. An interesting observation is that this stability condition is possible *without loss in accuracy.* On the practical side the most attractive feature of the new method is that for the (1,1) approximation, the numerical finite difference technique requires that we solve only one tridiagonal system at each step. Moreover, a (2,2) approximation, which delivers a higher accuracy, can also be derived; in this case the numerical finite difference technique requires that we solve either two successive tridiagonal systems or, equivalently, a (narrow) pentadiagonal system. The complete development of the method, its stability analysis along with the analysis of its accuracy and the examination of the wide angle capabilities of the (1,1) and (2,2) approximations are described in this paper.

2. Solution background

The wide angle 2-D wave equation was developed from the classical formulation of the three-dimensional Helmhotz equation in cylindrical coordinates (r, θ, z):

$$\frac{\partial^2 p}{\partial r^2} + \frac{1}{r}\frac{\partial p}{\partial r} + \frac{\partial^2 p}{\partial z^2} + k_0^2 n^2 p = 0. \tag{2.1}$$

In the above equation p represents the acoustic pressure, $k_0 = \omega/c_0$ where c_0 is a reference sound speed, $\omega = 2\pi f$, in which f is the frequency of the signal and finally $n = n(r,z) = c_0/c(r,z)$ is the index of refraction, in which $c(r,z)$ is the sound speed.

A standard transformation of the above equation is achieved by writing the pressure in the form [10]:

$$p(r,z) = u(r,z)v(r)$$

where the factor $v(r)$ represents a rapidly varying portion of the pressure and $u(r,z)$ is its modulation, a slowly varying function with respect to range. After neglecting small terms, making use of the far-field approximation ($k_0 r >> 1$), and rearranging the above equation we get the equation in u:

$$\frac{\partial^2 u}{\partial r^2} + 2ik_0\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial z^2} + (n^2 - 1)k_0^2 u = 0. \tag{2.2}$$

This new equation has been at the origin of the very successful small angle parabolic approximation technique, which consists of simply dropping the second order partial derivative with respect to r and integrating the resulting parabolic equation.

We define the operator

$$X = \frac{1}{k_0^2}\frac{\partial^2}{\partial z^2} + (n^2 - 1), \tag{2.3}$$

so that (2.2) reads,

$$\frac{\partial^2 u}{\partial r^2} + 2ik_0\frac{\partial u}{\partial r} + k_0^2 X u = 0. \tag{2.4}$$

The standard techniques for approximating the above equation, starting by approximately factoring the above operator as the product

$$\left[\frac{\partial}{\partial r} + ik_0 - ik_0 Q\right]\left[\frac{\partial}{\partial r} + ik_0 + ik_0 Q\right], \tag{2.5}$$

in which

$$Q \equiv \sqrt{1+X}. \tag{2.6}$$

Then the second term in this factorization is dropped to yield the so-called one-way outgoing wave equation:

$$u_r = (-ik_0 + ik_0\sqrt{1+X})u \tag{2.7}$$

The main effort in the literature has been to obtain a satisfactory approximation to the operator $\sqrt{1+X}$, and there have been a host of proposed techniques based on this. The standard parabolic approximation developed by Tappert [10] consists of using the approximation

$$\sqrt{1+X} \approx 1 + \frac{1}{2}X,$$

which yields the approximate equation from (2.7):

$$u_r = \frac{ik_0}{2}\left(n^2(r,z) - 1\right)u + \frac{i}{2k_0}u_{zz} \tag{2.8}$$

The above equation is then solved by either finite differences (method of lines) or using the Fast Fourier Transform, in which case the corresonding technique is labelled split-step Fourier transform. It is well known that the above split-step algorithm is capable of handling only narrow angle propation.

To relax the limitation of narrow angle propagation, a wide angle PE technique was first introduced by Claerbout [3], who used rational function approximations to the operator $\sqrt{1+X}$, of the form:

$$\sqrt{1+X} \approx \frac{1+pX}{1+qX}. \tag{2.9}$$

Claerbout used $p = 3/4$, and $q = 1/4$, but we keep arbitrary values for p, q for generality. Then (2.7) results in:

$$u_r = \left(-ik_0 + ik_0\frac{1+pX}{1+qX}\right)u, \tag{2.10}$$

which is a pseudo - partial-differential equation, referred to as the conventional wide angle wave equation.

Numerical methods for efficiently solving (2.10) based on a Crank-Nicolson type Implicit Finite Difference (IFD) scheme have been developed by Botseas, Lee, and Gilbert

[2]. The application of Crank-Nicolson brings (2.10) into a system of difference equations of the form

$$(I - \frac{1}{2}\Delta r L)u^{n+1} = (I + \frac{1}{2}\Delta r L)u^n, \qquad (2.11)$$

where,

$$L = -ik_0 + ik_0 \frac{1 + pX}{1 + qX}. \qquad (2.12)$$

There are three different ways of handling (2.11). In the first one, its two members are multiplied by $1 + qX$, assuming that $n^2(r, z)$ is range independent [9]. In the second approach the operator L is expanded in Taylor series where terms up to the degree 3 in X are maintained [4, 9]. Finally the third approach is to solve (2.11) by a scheme more accurate than Crank Nicolson [5]. Any of the above approaches will end up with a marching scheme of the form

$$Au^{n+1} = Bu^n + u_0^n + u_0^{n+1},$$

where u_0^n, u_0^{n+1}, are related to boundary information and where A and B are tridiagonal or pentadiagonal matrices.

To allow a comparison with our new scheme to be described next, we should point out that the narrow angle parabolic equation can accomodate angles of propagation up to 10^o. Approaches 1 and 2 of the wide angle wave equation can accomodate angles of propagation up to 23^o. The higher order finite difference scheme and the use of improved rational function coefficients of [5, 8] can accomodate angles as high as 40^o.

3. The new approach

In our new approach we regard the equation (2.4) as a second order ordinary differential equation with respect to the variable r. Therefore, the variable z will be dropped out in the remainder of the paper for convenience : $u(r)$ stands for $u(r, z)$. The difference between the standard techniques overviewed in the previous section and the new technique is that we do not approximate the square-root operator. Our approach starts by observing that locally, the formal solution to the equation (2.7) takes the form

$$u(r + \Delta r) = e^{-ik_0\Delta r} e^{ik_0\Delta r\sqrt{1+X}} u(r)^+ + e^{-ik_0\Delta r} e^{-ik_0\Delta r\sqrt{1+X}} u(r)^- \qquad (3.1)$$

where $u(r)^+$ and $u(r)^-$ are some initial conditions at the range r. The first term in the above solution is the outgoing wave and the second is the incoming wave. In this paper we will neglect back-scattering and therefore the second term will be dropped to yield the local solution

$$u(r + \Delta r) = e^{-\sigma} e^{\sigma\sqrt{1+X}} u(r) \tag{3.2}$$

in which we have set

$$\sigma \equiv ik_0 \Delta r.$$

Note that this is also a local solution of the one-way wave equation

$$u_r = (-ik_0 + ik_0\sqrt{1+X})u$$

which is obtained by neglecting the second factor in (2.5).

A standard way of solving the above equation is to use the approximation

$$\sqrt{1+X} \approx 1 + \frac{1}{2}X$$

which yields the standard two-dimensional narrow angle parabolic equation:

$$u_r = \left(\frac{1}{2}ik_0(n^2 - 1) + \frac{i}{2k_0}\frac{\partial^2}{\partial z^2}\right) u \equiv Lu.$$

This equation was introduced by Tappert [10]. However it represents accurately narrow angle propagation only. The approach taken here is to try to approximate the term $e^{\sigma\sqrt{1+X}}$ directly in an accurate way in order to accomodate higher angles of propagation.

We would like to derive a rational approximation for the term $e^{\sigma\sqrt{1+X}}$. In doing so we should set two important goals. The first is that the corresponding marching process should be easy to implement in a computer code and should not be too costly. The second goal is that the resulting formula be stable. Two rational function approximations denoted by Pade(1,1) and Pade (2,2) satisfying these requirements are described below. Before proceeding with their development, we introduce the function

$$G(\sigma, x) = e^{\sigma\sqrt{1+x}}. \tag{3.3}$$

This is a function of the real variable x, with the complex parameter σ. A Taylor expansion of the function G with respect to the variable x, about the point $x = 0$, yields,

$$
\begin{aligned}
G(\sigma,x) =& e^{\sigma}\left[1+\frac{\sigma}{2}x+\frac{\sigma(\sigma-1)}{4}\frac{x^2}{2!}+\frac{1}{8}(3\sigma-3\sigma^2+\sigma^3)\frac{x^3}{3!}\right. \\
&\left.+\frac{1}{16}(-15\sigma+15\sigma^2-6\sigma^3+\sigma^4)\frac{x^4}{4!}\right]+O(x^5)
\end{aligned}
\tag{3.4}
$$

3.1. The Pade(1,1) approximation

We look for an approximation to the function (3.3) of the form

$$
G_1(\sigma,x)=e^{\sigma}\frac{1+px}{1+qx}. \tag{3.5}
$$

The Pade (1,1) formula is obtained by matching the Taylor expressions of G and G_1. More precisely we will require that

$$
\frac{1+px}{1+qx}=1+\frac{\sigma}{2}x+\frac{\sigma(\sigma-1)}{4}\frac{x^2}{2!}+O(x^3) \tag{3.6}
$$

Moreover, for stability we impose the additional condition that the rational function (3.5) be of modulus one for real x. For this it suffices to ask that p and q be complex conjugate to each other. From (3.6) and this condition we easily find that

$$
p=\frac{1+\sigma}{4} \qquad q=\frac{1-\sigma}{4}
$$

which gives

$$
G_1(\sigma,x)=e^{\sigma}\frac{1+\frac{1+\sigma}{4}x}{1+\frac{1-\sigma}{4}x}. \tag{3.7}
$$

Observe that as required, for real x we have that $|G(\sigma,x)|=1$ since σ is purely imaginary. Furthermore, it can be seen that the error in the above approximation satisfies

$$
\|G(\sigma,x)-G_1(\sigma,x)\|=O(\sigma x^3).
$$

As a conseqence, as might be expected, when either $\sigma=0$ or $x=0$ the approximation is exact. This is not the case for the usual parabolic approximation which is only exact when $\sigma=0$.

3.2. The Pade(2,2) approximation

The Pade(2,2) rational approximation takes the form

$$
G_2(\sigma,x)=e^{\sigma}\frac{1+p_1x+p_2x^2}{1+q_1x+q_2x^2}. \tag{3.8}
$$

We now can match the Taylor expressions of G and G_2 up to the degree 4:

$$\begin{aligned}\frac{1+p_1x+p_2x^2}{1+q_1x+q_2x^2} =&1+\frac{\sigma}{2}x+\frac{\sigma(\sigma-1)}{4}\frac{x^2}{2!}+\frac{1}{8}(3\sigma-3\sigma^2+\sigma^3)\frac{x^3}{3!} \\ &+\frac{1}{16}(-15\sigma+15\sigma^2-6\sigma^3+\sigma^4)\frac{x^4}{4!}+O(x^5)\end{aligned} \tag{3.9}$$

For stability we impose again that the rational function (3.8) be of modulus one for real x by requiring that p_i and q_i be complex conjugate to each other, for $i=1,2$. After some algebraic calculations we finally arrive at the expressions,

$$p_1=\frac{3+\sigma}{4}, \qquad p_2=\frac{\sigma^2+6\sigma+3}{48}$$

$$q_1=\frac{3-\sigma}{4}, \qquad q_2=\frac{\sigma^2-6\sigma+3}{48}$$

In other words

$$G_2(\sigma,x)=e^{\sigma}\frac{1+\frac{3+\sigma}{4}x+\frac{\sigma^2+6\sigma+3}{48}x^2}{1+\frac{3-\sigma}{4}x+\frac{\sigma^2-6\sigma+3}{48}x^2} \tag{3.10}$$

Here the error is $O(\sigma^2x^4)$.

4. Numerical Solution

Replacing the approximation G_1 for the exponentional term $exp\ (\sigma\sqrt{1+X})$ in (3.1) we obtain the formal expression for marching one step

$$u(r+\Delta r,z)=\frac{1+\frac{1+\sigma}{4}X}{1+\frac{1-\sigma}{4}X}u(r,z)$$

Numerically this leads to an implicit integration scheme of the form:

$$\left(1+\frac{1-\sigma}{4}X_h\right)u^{n+1}=\left(1+\frac{1+\sigma}{4}X_h\right)u^n \tag{4.1}$$

Here X_h represents a centered difference approximation to the partial differential operator X with respect to the variable z. The discretization is taken for the variable r equal to $r+\frac{1}{2}\Delta r$.

Similarly, the Pade(2,2) approximation leads to the integration scheme

$$\left(1+\frac{3-\sigma}{4}X_h+\frac{\sigma^2-6\sigma+3}{48}X_h^2\right)u^{n+1}=\left(1+\frac{3+\sigma}{4}X_h+\frac{\sigma^2+6\sigma+3}{48}X_h^2\right)u^n \tag{4.2}$$

Computationally, the two marching schemes can be performed by resorting only to solutions of tridiagonal systems and multiplications by tridiagonal matrices. More precisely, each step of Pade(1,1) requires solving one tridiagonal system and one multiplication of a vector by a tridiagonal matrix. Concerning Pade(2,2) the matrix on the left hand side of (4.2) is a banded matrix of bandwidth 5, i.e., it is a narrow pentadiagonal matrix. Linear systems involving such matrices can be efficiently solved by Gaussian elimination. Moreover, an alternative is to factor the left hand side of (4.2) as the product of two linear terms in X_h in which case the solution of the system (4.2) can be obtained as the result of solving two successive tridiagonal systems. In other words, in addition to the multiplication of a vector by a pentadiagonal matrix, the scheme Pade(2,2) requires solving either one narrow pentadiagonal system, or two successive tridiagonal systems.

5. Numerical Tests

In order to test the accuracy of our schemes and to determine the maximum size of propagation angles we have run a few tests using the reference solution constructed by St Mary and Lee [9]:

$$\Phi(r,z) = \frac{i}{2z_h} \sum_{j=0}^{\infty} sin\left(kz_0\sqrt{1-a_j^2}\right) sin\left(kz\sqrt{1-a_j^2}\right) H_0^{(1)}(ka_j r). \tag{5.1}$$

where a_j satisfies

$$a_j = \sqrt{1 - \left(\frac{(j+1/2)\pi}{kz_h}\right)^2}, \tag{5.2}$$

which satisfies the Helmhotz equation with the source term

$$\Phi_{rr} + \frac{1}{r}\Phi_r + \Phi_{zz} + k^2\Phi = -\delta(z - z_0)\frac{\delta(r)}{2\pi r} \tag{5.3}$$

where δ is the Dirac function, and z_h is the bottom depth. The term a_j in the radical is determined by (5.2) and $j + 1$ indicates the number of the propagating mode. From this solution the size of the angle of propagation can be tabulated [9]. We use a source frequency of 50Hz in a homogeneous medium to construct the mode-angle table, a section of which is displayed in Table 1 for reference.

We accept the solution if the difference between it and the exact solution is within one dB. This accuracy criterion is suitable for measuring how wide the angle of propagation is. The results are tabulated in Table 2. Additional inputs used include: source depth = 300m, water depth = 400 m, receiver depth = 100m, and maximum range = 10km. The initial field was generated from the exact mode solution.

Mode number j	Angle (degrees)
14	32.95
15	35.54
16	38.22
.. ..	.. ..
21	53.72
22	57.54
23	61.79

Table 1: Mode-Angle relationship.

Method	Number of modes	Angle (degrees)
Pade(1,1)	16	35.54
Pade(2,2)	23	57.54

Table 2: Wide angle capability.

5.1. Pade(1,1) Test Results

Formula (4.1) was used to predict the long range wave propagation by taking advantage of the wide angle capability. Using the mode solution as a reference, our experiments show that up to 15 propagating modes, the Pade(1,1) solution agrees well with the exact solution. For 16 propagating modes, the maximum difference between the Pade(1,1) result and the mode solution is approximately 1 dB, as is shown in Figure 1.

When we used 17 propagating modes, the maximum difference exceeds 1dB and was therefore rejected in agreement with our criterion. Note that the solution is still usable, since the large error of 1dB only occurs in some spots at the end of the marching process. As a result our technique can handle up to 15 propagating modes, which corresponds to angles as wide as 35 degrees.

5.2. Pade(2,2) Test Results

Similarly, formula (4.2) has heen used in the same example and for the same purpose as above, i.e., for estimating maximum propagation angles that it can handle. Figure 2 shows that there is a satisfactory agreement between the Pade(2,2) approximate solution and the exact solution as provided by the modal expansion approach, for up to 23 propagating modes. The same criterion of accepting a maximum error of 1dB has been applied. To compare the solutions provided by Pade(1,1) and Pade(2,2) we also plotted the answer provided by Pade(2,2) for 16 propagating modes. As is shown in Figure 3, Pade(2,2) handles the 16 propagating modes with great accuracy and the approximation is hardly even distinguishable from the exact solution. Thus, Pade(2,2) is far more powerful than Pade(1,1) but each of its steps costs twice as much as a step of Pade(1,1). However, a fair comparison should also take into account the fact that we may need fewer steps with Pade(2,2) than with Pade(1,1) since with the higher accuracy we can afford a larger step-size.

6. Conclusion

An important goal in computational methods for predicting long range ocean acoustic propagation is efficiency and speed. The advantage of the methods introduced in this paper is that the solution scheme is accurate enough to be able to handle much wider angles than existing techniques having similar cost per step. Our Pade(1,1) can accomodate a 35 degree propagation angle, while our Pade(2,2) scheme can accomodate as high an angle as 54 degrees. Most important is the fact that unconditional stability is guaranteed in most environmental conditions.

An adaptation of this work to three-dimensional problems has already been developed by Lee, Saad and Schultz [7] and the numerical results shown there are very promising. Work remains to be done to improve the three-dimensional approximation to obtain a very wide angle solution method.

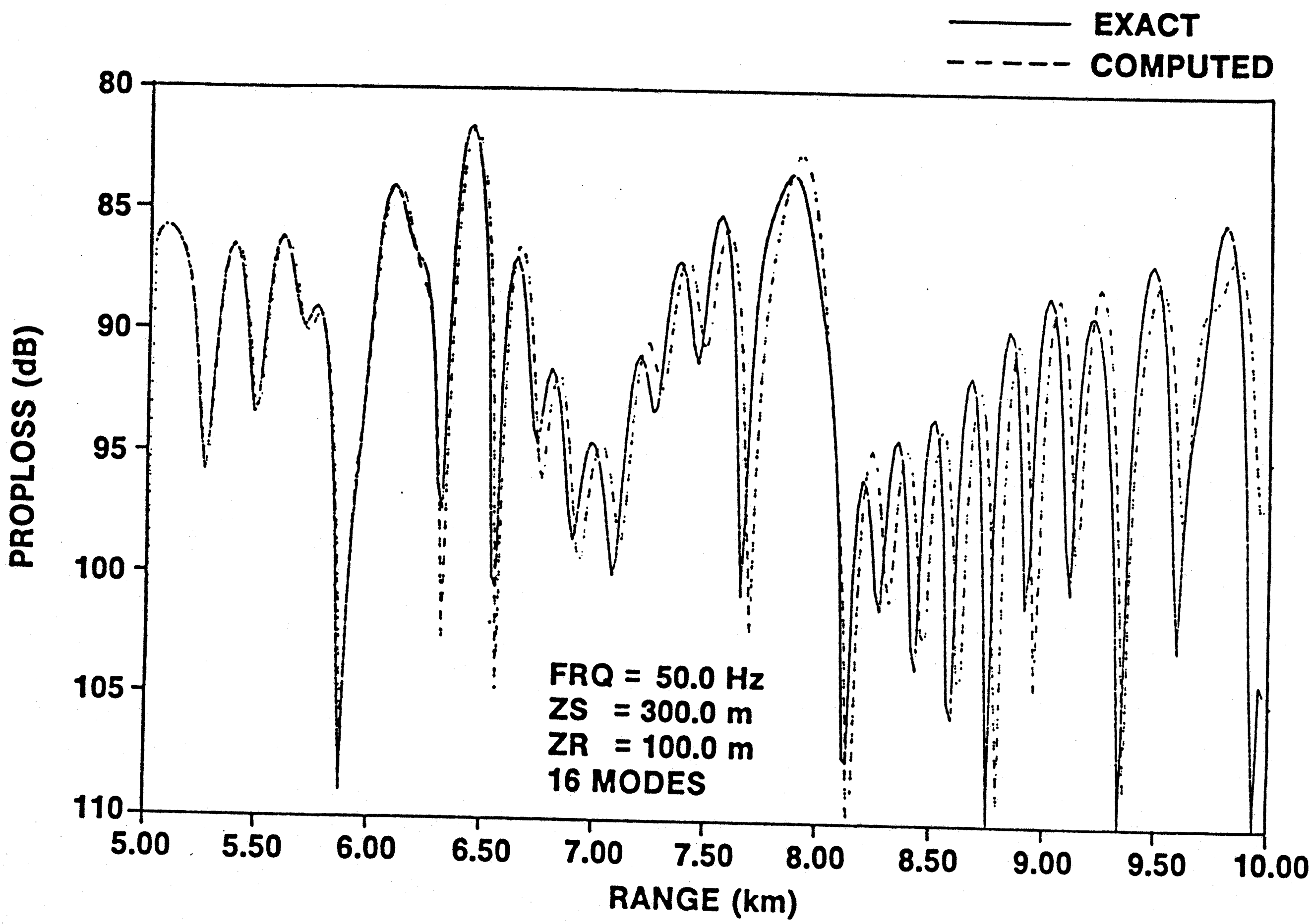

Figure 1: Pade(1,1) test results for 16 propagating modes. Solid line = exact solution, dashed line = computed solution.

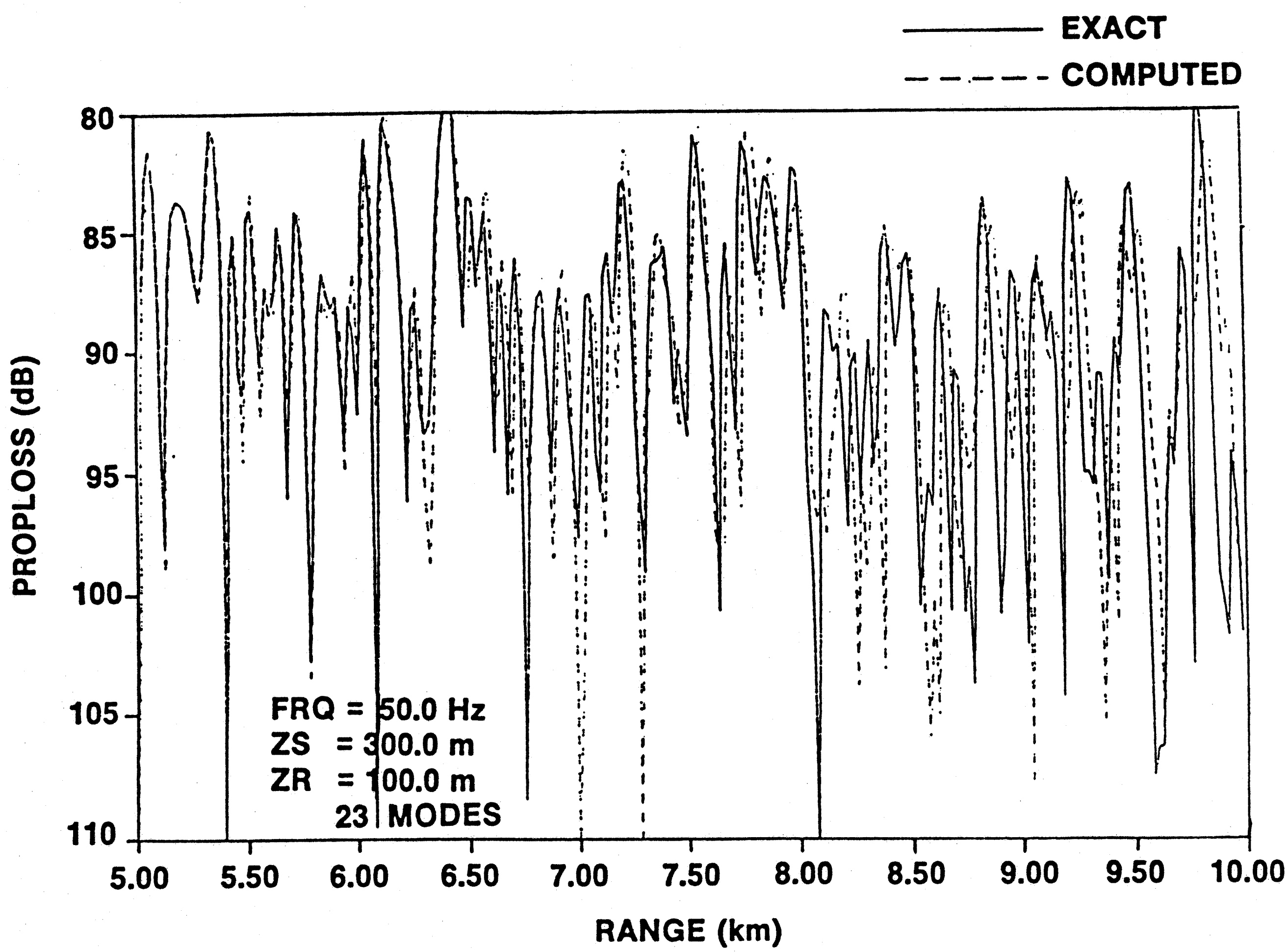

Figure 2: Pade(2,2) test results for 23 propagating modes. Solid line = exact solution, dashed line = computed solution.

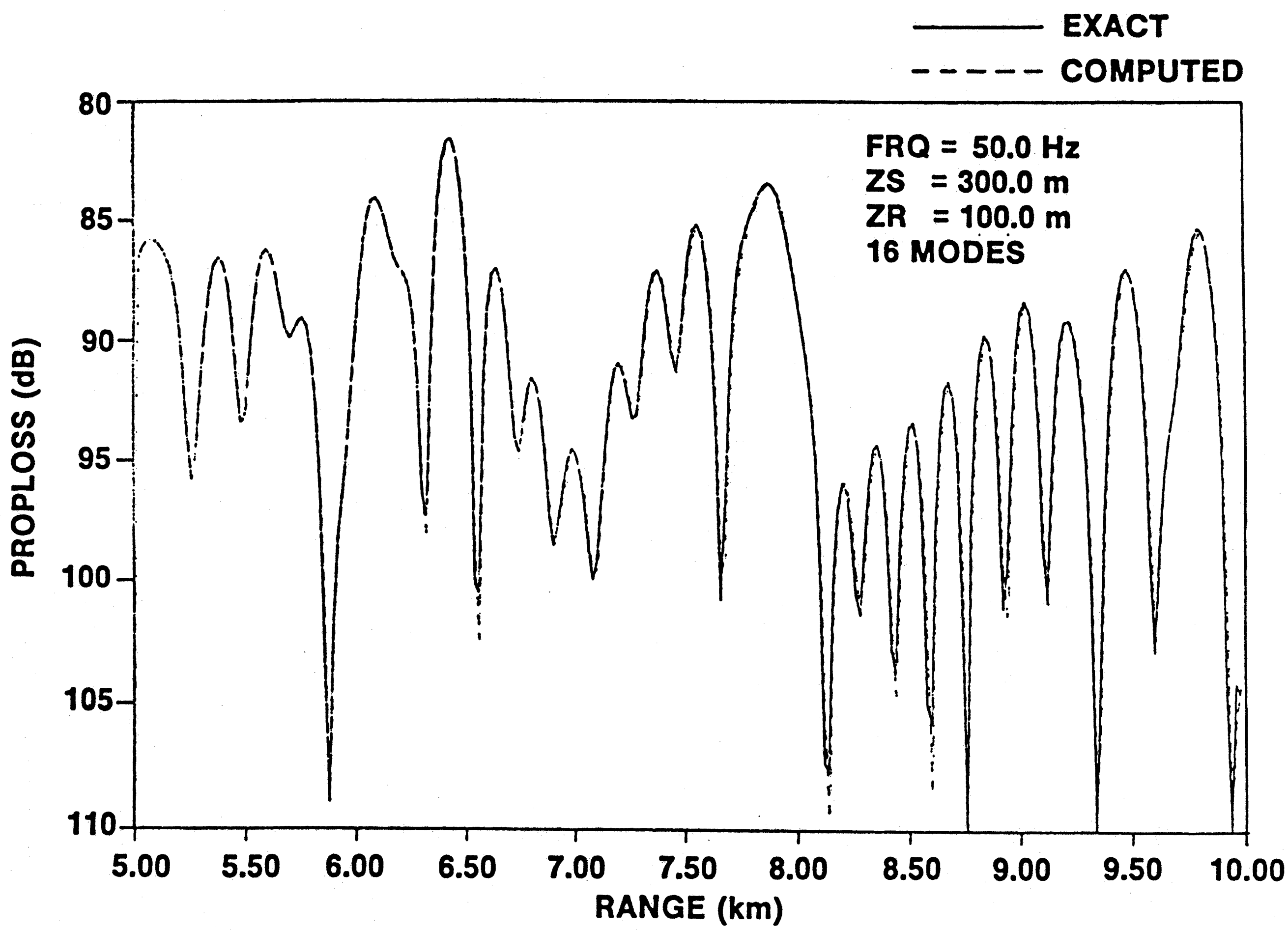

Figure 3: Pade(2,2) test results for 16 propagating modes. Solid line = exact solution, dashed line = computed solution.

Acknowledgement The authors would like to thank Prof. Donald St. Mary for his valuable help and for allowing us to use some of his codes.

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