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of iterative parabolic equations**

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On the decomposition of the fundamental solution of the Helmholtz equation via solutions of iterative parabolic equations

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Abstract. Recently it was shown that the solution of the Helmholtz equation can be approximated by a series over the solutions of iterative parabolic equations. An extension of the fundamental solution of the Helmholtz equation via the solution of the iterative parabolic equations is considered. Initial conditions are derived which are consistent with the iterative parabolic equations. The derived conditions can be used to model the wave field generated by a point source.

Keywords: Helmholtz equation, paraxial approximation, multiple scales, iterative parabolic equations, wide-angle parabolic equations, self-starter, Pattern solver tool

1. Introduction

The parabolic equations method is currently one of the most important tools for the simulation of wave propagation in different media [1, 2]. In pioneering works wide-angle parabolic equations (PEs) are usually derived from Padé approximations of an operator square root resulting from the formal factorization of the Helmholtz equation [3, 4]. The solution of such equations allows to simulate one-way wave propagation both efficiently and accurately [2]. It is known that both the aperture of a PE (i.e., its capability to handle wide-angle effects) and the stability of its solution strongly depends on the choice of the Cauchy data in the respective initial-boundary value problems [2, 5, 6] (often referred to as starters in the PE theory). Various techniques have been used in the literature for the design of starters, including analytical methods, normal mode theory, ray theory and the so-called self-starter approach [2, 5, 6].

Recently Trofimov [7] proposed a new approach to the PE theory. Trofimov's derivation is based on the method of multiple scales [7], and it leads to a system of so-called iterative PEs, where the solution of the j -th equation is used to calculate the input term of the $j + 1$ -th equation (thus, higher order equations can be considered as a correction to lower order ones). This approach was further developed in [8], and in [9] it was also shown that it can be extended to the case of nonlinear media (leading to first wide-angle parabolic approximations to a nonlinear equation). Despite considerable success in the development of

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the method, no consistent starters for iterative PEs have been developed so far (in previous work we have mostly used the starters for standard wide-angle PEs, e.g., those described in [2]). This present study aims to close this gap.

In our work we derive initial conditions (or starters) for iterative PEs that can be used to simulate the wavefield generated by a point source (the case of distributed sources is also covered by our derivation). The starter is obtained by using the same asymptotic expansion for the fundamental solution of the Helmholtz equation as used in [7] for the derivation of iterative PEs. This expansion is interesting in itself, because to our knowledge the counterpart of this fundamental solution has not been considered in the 'PE world' so far.

2. Helmholtz equation and iterative parabolic approximations

In this work we consider the Helmholtz equation [2] describing an acoustic field produced by a point source located at $x = 0$, $y = 0$, $z = 0$ in a 3D homogeneous medium

$$u_{xx} + u_{yy} + u_{zz} + k^2 u = \delta(x)\delta(y)\delta(z). \quad (1)$$

The solution $u = u(x, y, z)$ to Eq. (1) is the sound pressure, and k denotes the wavenumber (the ratio of the angular frequency to the sound speed). In acoustics the variable z usually denotes the depth, x is the range along some acoustic path, and y is the transverse horizontal direction. Our goal here is to simulate the paraxial propagation of sound along the x axis.

Such kind of wave propagation in a preferred direction can be efficiently described by so-called *parabolic equations (PEs)* that can be derived either via a pseudo-differential one-way Helmholtz equation or using a direct multiscale approach. In this study we focus on the second approach introduced 2013 by Trofimov [7] in the context of 2D propagation in ocean acoustics. It was later generalized to the 3D case by Petrov [10]. In the sequel we briefly outline the idea and the main results of the approach of Trofimov [7].

We start the derivation of the iterative PEs by introducing slow variables with the so-called *parabolic scaling* $X = \epsilon x$, $Y = \epsilon^{1/2} y$ and $Z = \epsilon^{1/2} z$, and the fast variable $\eta = (1/\epsilon) \theta(X, Y, Z)$.

Following the idea of the method of multiple scales [11] we assume that

$$k^2 = k_0^2 + \epsilon \nu(X, Y, Z), \quad (2)$$

and seek the solution of Eq. (1) in the form

$$u = u_0(X, Y, Z, \eta) + \epsilon u_1(X, Y, Z, \eta) + \dots \quad (3)$$

Next, we replace the derivatives in (1) using the chain rule

$$\frac{\partial}{\partial x} \rightarrow \epsilon \left(\frac{\partial}{\partial X} + \frac{1}{\epsilon} \theta_X \frac{\partial}{\partial \eta} \right), \quad \frac{\partial}{\partial y} \rightarrow \epsilon^{1/2} \left(\frac{\partial}{\partial Y} + \frac{1}{\epsilon} \theta_Y \frac{\partial}{\partial \eta} \right), \quad \frac{\partial}{\partial z} \rightarrow \epsilon^{1/2} \left(\frac{\partial}{\partial Z} + \frac{1}{\epsilon} \theta_Z \frac{\partial}{\partial \eta} \right).$$

Substituting (2) and (3) into (1), collecting the terms of the same orders in ϵ and solving the resulting equations one by one we finally obtain the following series for $u(x, z)$:

$$u(x, y, z) = \exp(ik_0x) \sum_{j=0}^{\infty} \mathcal{A}_j(x, y, z) = \exp(ik_0X/\epsilon) \sum_{j=0}^{\infty} \epsilon^j A_j(X, Y, Z). \quad (4)$$

The amplitudes $\mathcal{A}_j(x, y, z)$, in the series (4) can be obtained (cf. [7, 10]) from the following system of iterative parabolic equations:

$$2ik_0 \mathcal{A}_{j,x} + \mathcal{A}_{j,yy} + \mathcal{A}_{j,zz} + \nu \mathcal{A}_j + \mathcal{A}_{j-1,xx} = 0, \quad j = 0, 1, 2, \dots, \quad (5)$$

where we set $A_{-1}(x, y, z) \equiv 0$. Note that by definition we have $\mathcal{A}_j(x, y, z) \equiv \epsilon^j A_j(X, Y, Z)$.

The approximation of $u(x, y, z)$ obtained by taking into account only the first $N + 1$ terms $A_0(x, y, z), \dots, A_N(x, y, z)$ of the series (4) is called *N-th order iterative parabolic approximation*. The iterative parabolic equations (5) should be solved one by one, and the solution of the n -th equation is used as the input for the $n + 1$ -th equation.

It is interesting to note that a system similar to (5) first appeared 1986 in the work of Grikurov and Kiselev [12]. They studied the accuracy of the solution given by a narrow-angle PE in ray coordinates, and derived a simplified version of (5) in order to estimate the contribution of the high-order terms.

3. Decomposition of the fundamental solution of the Helmholtz equation

The 3D Helmholtz equation (1) possess a fundamental solution

$$\mathcal{F}_3(x, y, z) = \frac{e^{ikR}}{4\pi R}, \quad (6)$$

where $R = \sqrt{x^2 + y^2 + z^2}$.

Let us now define F_3 as $F_3(X, Y, Z) = \mathcal{F}_3(X/\epsilon, Y/\sqrt{\epsilon}, Z/\sqrt{\epsilon})$. Clearly, the terms in the expansion of $F_3(X, Y, Z) \cdot e^{-ikX/\epsilon}$ over the powers of ϵ must be equal to the respective terms of the series $\sum_{j=0}^{\infty} \epsilon^j A_j(X, Y, Z)$. The former expansion reads

$$\begin{aligned} \frac{e^{ik\frac{X}{\epsilon} \left(\sqrt{1 + \frac{\epsilon(Y^2 + Z^2)}{X^2}} - 1 \right)}}{4\pi\frac{X}{\epsilon} \sqrt{1 + \frac{\epsilon(Y^2 + Z^2)}{X^2}}} &= \frac{\epsilon}{4\pi X} e^{\frac{1}{2}ik\frac{Y^2 + Z^2}{X}} \left(1 + \epsilon \left(-\frac{1}{2} \frac{(Y^2 + Z^2)}{X^2} - \frac{1}{8} ik \frac{(Y^2 + Z^2)^2}{X^3} \right) \right. \\ &\left. + \epsilon^2 \left(\frac{3}{8} \frac{(Y^2 + Z^2)^2}{X^4} - \frac{1}{128} k^2 \frac{(Y^2 + Z^2)^4}{X^6} + \frac{1}{8} ik \frac{(Y^2 + Z^2)^3}{X^5} \right) + \epsilon^3(\dots) \right). \quad (7) \end{aligned}$$

Hence we obtain the following expressions for the free-space solutions of the iterative PEs (5) in rescaled variables X, Y, Z

$$A_0(X, Y, Z) = \frac{\epsilon}{4\pi X} e^{\frac{1}{2}ik\frac{Y^2 + Z^2}{X}},$$

$$\begin{aligned}
A_1(X, Y, Z) &= \frac{\epsilon}{4\pi X} e^{\frac{1}{2}ik\frac{Y^2+Z^2}{X}} \left(-\frac{1}{2} \frac{(Y^2 + Z^2)}{X^2} - \frac{1}{8} ik \frac{(Y^2 + Z^2)^2}{X^3} \right), \\
A_2(X, Y, Z) &= \frac{\epsilon}{4\pi X} e^{\frac{1}{2}ik\frac{Y^2+Z^2}{X}} \left(\frac{3}{8} \frac{(Y^2 + Z^2)^2}{X^4} - \frac{1}{128} k^2 \frac{(Y^2 + Z^2)^4}{X^6} + \frac{1}{8} ik \frac{(Y^2 + Z^2)^3}{X^5} \right), \dots \quad (8)
\end{aligned}$$

Let us stress the fact that the solutions of iterative PEs (8) correspond to the fundamental solution of the Helmholtz equation, i.e., to the wavefield produced by a point source. Eq. (8) implies that the j -th term of the series $\sum_{j=0}^{\infty} \epsilon^j A_j(X, Y, Z)$ is of the order ϵ^{j+1} , not ϵ^j (e.g., the term A_0 is of the order ϵ).

Next, rewriting the solutions (8) in physical variables x, y, z , we obtain

$$\begin{aligned}
\mathcal{A}_0(x, y, z) &= \frac{1}{4\pi x} e^{\frac{1}{2}ik\frac{y^2+z^2}{x}}, \\
\mathcal{A}_1(x, y, z) &= \frac{1}{4\pi x^2} e^{\frac{1}{2}ik\frac{y^2+z^2}{x}} \left(-\frac{1}{2} \frac{(y^2 + z^2)}{x} - \frac{1}{8} ik \frac{(y^2 + z^2)^2}{x^2} \right), \\
\mathcal{A}_2(x, y, z) &= \frac{1}{4\pi x^3} e^{\frac{1}{2}ik\frac{y^2+z^2}{x}} \left(\frac{3}{8} \frac{(y^2 + z^2)^2}{x^2} + \frac{1}{8} ik \frac{(y^2 + z^2)^3}{x^3} - \frac{1}{128} k^2 \frac{(y^2 + z^2)^4}{x^4} \right), \\
\mathcal{A}_3(x, y, z) &= \frac{1}{4\pi x^4} e^{\frac{1}{2}ik\frac{y^2+z^2}{x}} \left(-\frac{5}{16} \frac{(y^2 + z^2)^3}{x^3} - \frac{15}{128} ik \frac{(y^2 + z^2)^4}{x^4} + \frac{3}{256} k^2 \frac{(y^2 + z^2)^5}{x^5} \right. \\
&\quad \left. + \frac{1}{3072} ik^3 \frac{(y^2 + z^2)^6}{x^6} \right), \dots \quad (9)
\end{aligned}$$

Remark 1. It might seem confusing that for purely real values of the medium wavenumber k the solutions of the iterative PEs (9) are not even square-integrable functions. However, in physical applications (e.g., in underwater acoustics) the waves are always attenuated by the media (e.g., the water column, the seabed), and therefore $\text{Im}(k) > 0$. For arbitrarily small yet positive $\text{Im}(k)$ all solutions (9) belong to $C([0, \infty), L^2(\mathbb{R}^2))$. However, for a lossless medium with $\text{Im}(k) = 0$ the solutions (9) must be considered in a distributional sense.

Let us derive a general expression for $A_n(X, Y, Z)$. We start with introducing the following quantities

$$P = X^2 + Y^2,$$

$$W = ik \frac{X}{\epsilon} \left(\sqrt{1 + \frac{\epsilon(Y^2 + Z^2)}{X^2}} - 1 \right).$$

Our goal is to obtain the expansion for the reduced fundamental solution

$$\bar{F}(X, Y, Z, \epsilon) = 4\pi \frac{X}{\epsilon} F_3(X, Y, Z) e^{-ikX/\epsilon} = e^W \left(1 + \frac{\epsilon P}{X^2} \right)^{-1/2}$$

over the powers of ϵ . This objective can be achieved by computing all derivatives $d^n \bar{F}/d\epsilon^n|_{\epsilon=0}$. One can easily verify that

$$\frac{d\bar{F}}{d\epsilon} = \bar{F} \cdot V, \quad (10)$$

where

$$V = W' - \frac{1}{2} \frac{P}{X^2} \left(1 + \frac{\epsilon P}{X^2}\right)^{-1}$$

(hereafter primes denote derivatives w.r.t. the scaling parameter ϵ).

Computing the second and the third derivatives of \bar{F} w.r.t. ϵ that have the form

$$\frac{d^2 \bar{F}}{d\epsilon^2} = F(V^2 + V'),$$

and

$$\frac{d^3 \bar{F}}{d\epsilon^3} = F(V^3 + 3VV' + V''),$$

we observe that in general

$$\frac{d^n \bar{F}}{d\epsilon^n} = \bar{F} S_n(V), \quad (11)$$

where the expressions $S_n(V)$ containing products of V and their derivatives can be obtained recursively by the formula

$$S_n(V) = V \cdot S_{n-1}(V) + S'_{n-1}(V), \quad n = 1, 2, 3, \dots,$$

starting with $S_0(V) = 1$.

Since

$$V^{(n)} = W^{(n+1)} - \frac{1}{2} \left(\frac{P}{X^2}\right)^{n+1} (-1)^n n! \left(1 + \frac{\epsilon P}{X^2}\right)^{-(n+1)},$$

it only remains to compute $W^{(n+1)}$. The calculation is straightforward (yet tedious), and we present here only the resulting formula

$$W^{(n)} = \frac{-ikX}{\epsilon^{n+1}} (-1)^n n! + \sum_{j=0}^n \frac{ikX}{\epsilon^{n+1-j}} (-1)^{n-j} (n-j)! \left(1 + \frac{\epsilon P}{X^2}\right)^{1/2-j} \left(\frac{P}{X^2}\right)^j \frac{(-1)^{j-1}}{2^j} (2j-3)!!, \quad (12)$$

where we used the notation of the double factorial $!!$. Note that we actually need the formula for $V^{(n)}|_{\epsilon=0}$. Using Eq. (12) one can easily show that it can be written as

$$V^{(n)}|_{\epsilon=0} = -\frac{1}{2}(-1)^n n! \left(\frac{P}{X^2}\right)^{n+1} + \frac{ikX}{2^{n+1}} \left(\frac{P}{X^2}\right)^{n+1} (2n-1)!! \sum_{j=0}^n \frac{(-1)^j}{n+1-j} \binom{n}{j}. \quad (13)$$

The terms of the expansion of \bar{F} can therefore be easily computed by the formulae Eq. (11) and Eq. (13). In order to summarize all the results of our derivation we formulate the following theorem.

Theorem 1. *The general formula for the terms in the expansion (7) can be written as*

$$\mathcal{A}_j(x, y, z) = \frac{1}{4\pi x} e^{\frac{1}{2}ik\frac{y^2+z^2}{x}} \frac{S_j(v)}{j!}, \quad (14)$$

where $S_j(v) = (v^0 + D)^j \mathbf{1}$, and D is a formal differential operator defined by the formula $Dv^{(n)} = v^{(n+1)}$ (it is also assumed that D is linear, and that it satisfies the Leibniz rule). The functions $v^{(n)}(x, y, z)$ are given by the following formula

$$v^{(n)}(x, y, z) = -\frac{1}{2}(-1)^n n! \frac{(y^2 + z^2)^{n+1}}{x^{2(n+1)}} + \frac{ikx}{2^{n+1}} \frac{(y^2 + z^2)^{n+1}}{x^{2(n+1)}} (2n-1)!! \sum_{j=0}^n \frac{(-1)^j}{n+1-j} \binom{n}{j}. \quad (15)$$

Remark 2. Note that $\mathcal{A}_j(x, y, z) = \frac{1}{4\pi x^{j+1}} e^{\frac{1}{2}ik\frac{y^2+z^2}{x}} P_{2j}\left(\frac{y^2+z^2}{x}\right)$, where $P_{2j}(q)$ is a polynomial of degree $2j$.

4. Cauchy data for iterative PEs that corresponds to a point source

It is not immediately obvious what Cauchy data (i.e., initial conditions, or ICs) for the equations (5) correspond to the solutions (9). Indeed, it is not easy to see what is the limit of these expressions for $x \rightarrow 0$. In this section we guess the correct answer to this question by using some non-rigorous generalizations of the formulae for low-order terms in the expansion (4). Clearly, the derivation below cannot be considered as a formal proof of the final result (it is postponed until the next section). Nevertheless, we invite our readers to follow the course of our study.

Our first step is a lemma that can be easily proven using the standard formula for the fundamental solution of the heat equation (see, e.g., [13]) and the Duhamel's principle.

Lemma 4.1. *The function $\mathcal{A}_0(x, y, z)$ given by Eq. (9) is the solution of the Cauchy problem for the parabolic equation*

$$2ik_0 \mathcal{A}_{0,x} + \mathcal{A}_{0,yy} + \mathcal{A}_{0,zz} = -\delta(x, y, z), \quad x > 0,$$

with zero initial condition at $x = 0$. It can also be considered as a solution of the Cauchy problem

$$\begin{cases} 2ik_0 \mathcal{A}_{0,x} + \mathcal{A}_{0,yy} + \mathcal{A}_{0,zz} = 0, & x > 0, \\ \mathcal{A}_0|_{x=0} = -\delta(y, z). \end{cases} \quad (16)$$

Since the functions \mathcal{A}_j are distributions in y, z at $x = 0$, we can investigate their behavior by performing a smoothing in y, z -directions by a convolution with the Gaussian kernel function

$$G(y, z) = \frac{1}{\pi\sigma} e^{-\frac{y^2+z^2}{\sigma}}. \quad (17)$$

Indeed, once we replace the right-hand side in Eq. (1) by $\delta(x)G(y, z)$, its solution will be smeared to

$$\mathcal{F}_3 * G = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathcal{F}_3(x, \xi, \eta) G(y - \eta, z - \xi) d\eta d\xi$$

(note that symbol $*$ denotes the convolution in y and z directions only). Clearly, the respective solutions of the iterative parabolic equations (9) will also be smeared into $\mathcal{A}_j * G$. One can easily verify that

$$\begin{aligned} \mathcal{A}_0 * G|_{x=0} &= e^{-\frac{y^2+z^2}{\sigma}} \frac{i}{2\pi k\sigma} = \frac{i}{2k} G, \\ \mathcal{A}_1 * G|_{x=0} &= e^{-\frac{y^2+z^2}{\sigma}} \frac{i}{\pi k^3 \sigma^2} \left(1 - \frac{y^2+z^2}{\sigma}\right) = \frac{i}{2k} \left(-\frac{1}{2} \frac{\Delta}{k^2}\right) G, \\ \mathcal{A}_2 * G|_{x=0} &= e^{-\frac{y^2+z^2}{\sigma}} \frac{3i}{\pi k^5 \sigma^3} \left(2 - 4 \left(\frac{y^2+z^2}{\sigma}\right) + \left(\frac{y^2+z^2}{\sigma}\right)^2\right) = \frac{i}{2k} \left(\frac{3}{8} \frac{\Delta^2}{k^4}\right) G, \\ \mathcal{A}_3 * G|_{x=0} &= \dots = \frac{i}{2k} \left(-\frac{5}{16} \frac{\Delta^3}{k^6}\right) G, \dots, \end{aligned} \quad (18)$$

with the 2D Laplace operator $\Delta = \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$.

Now passing to the limit $\sigma \rightarrow 0$ we observe that

$$\mathcal{A}_j|_{x=0} = \frac{i}{2k} (-1)^j C_j \frac{\Delta^j}{k^{2j}} (\delta(y)\delta(z)), \quad (19)$$

and the coefficients are given by $C_0 = 1, C_1 = 1/2, C_2 = 3/8, C_3 = 5/16, \dots$. Although initially we failed to recognize the underlying formula for this sequence, four terms were sufficient to recover it using the 'Pattern Solver tool' [14]. It turned out to be

$$C_j = \frac{\binom{2j}{j}}{4^j}, \quad j = 1, 2, 3, \dots \quad (20)$$

Note that this sequence consists of the Taylor series coefficients for the function $1/\sqrt{1+x}$ (up to a sign). In turn, this observation leads to the following insightful equality

$$\sum_{j=0}^{\infty} \mathcal{A}_j|_{x=0} = \frac{i}{2k} \sum_{j=0}^{\infty} (-1)^j \frac{\binom{2j}{j}}{4^j} \frac{\Delta^j}{k^{2j}} (\delta(y)\delta(z)) = \frac{i}{2} \frac{1}{\sqrt{k^2 + \Delta}} (\delta(y)\delta(z)). \quad (21)$$

This quantity can be considered as a formal initial condition for a pseudo-differential PE (i.e., to a one-way counterpart for the Helmholtz equation (1)) corresponding to the point-source input term in Eq. (1).

Of course, this condition is in no way suitable for practical computations (one should subject it to a smoothing procedure before using in a numerical scheme), yet it led the authors of the present study to a clear and simple idea of a formal derivation of Eq. (19). A formula similar to (21) was also derived by Collins in his study on the self-starter for standard wide-angle parabolic equations [5].

5. Formal derivation of ICs for iterative PEs

In the previous section the way we guessed the final result was outlined. Once it was obtained, a formal proof was also easy to establish. We start with a more rigorous derivation of the formula (21). Let us first rewrite the Helmholtz equation (1) in the following form

$$\frac{\partial^2 u}{\partial x^2} + M^2 u = -\delta(x)\Omega, \quad (22)$$

where $M^2 = k^2 + \Delta^2$, and $\Omega = \delta(y)\delta(z)$. For $x > 0$ the solution of (22) can be formally written as

$$u(x, y, z) = \frac{i}{2M} e^{iMx}\Omega = \frac{i}{2\sqrt{k^2 + \Delta}} e^{i\sqrt{k^2 + \Delta}x} (\delta(y)\delta(z)). \quad (23)$$

By setting $x = 0$ in the last formula we formally obtain

$$u(x, y, z)|_{x=0} = \frac{i}{2\sqrt{k^2 + \Delta}} (\delta(y)\delta(z)), \quad (24)$$

and this formula coincides with Eq. (21).

Using Eq. (24) we can easily prove (19), and, correspondingly, a more general formula for a smoothed IC

$$\mathcal{A}_j * G|_{x=0} = \frac{i}{2k} (-1)^j \frac{\binom{2j}{j}}{4^j} \frac{\Delta^j}{k^{2j}} G.$$

In order to reestablish Eq. (19) we must rewrite the operator in Eq. (24) in rescaled variables. Indeed,

$$\Delta = \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \epsilon \left(\frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2} \right) = \epsilon \tilde{\Delta},$$

and therefore the operator in Eq. (24) can be formally expanded as

$$\frac{1}{\sqrt{\epsilon \tilde{\Delta} + k^2}} = \frac{i}{2k} \sum (-1)^j \frac{\binom{2j}{j}}{4^j} \frac{\tilde{\Delta}^j}{k^{2j}} \epsilon^j,$$

and thus the coincidence between the terms in expansion of $u(x, y, z)|_{x=0}$ and terms of the same powers of ϵ in Eq. (7) is established.

6. Concluding remarks

In this study we derived the solution of iterative parabolic equations (IPEs) that corresponds to the fundamental solution of the Helmholtz equation. In a sense, we obtained the counterpart of the self-starter (see [5]) for the IPE theory.

On the practical side this result yields the initial conditions for the solution of the Cauchy problem for IPEs that allow to simulate a wavefield produced by a point source (i.e., to approximate the solution of the Helmholtz equation with the delta input term).

In many problems of underwater acoustics it would be useful to construct a starter that is formed by vertical normal modes in z (in this case, e.g., only waterborne modes can be retained) but omnidirectional in the horizontal plane. This will be accomplished in future work.

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