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Improvements to Layer Matrix Methods

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Abstract. The problem of numerical instabilities at high frequencies is solved for the case of a source of $P-SV$ waves buried in a layered halfspace. The solution is to compute the high frequency layer matrices by multiplication of low frequency layer matrices. It is only required to compute the problematic exponential terms for a small frequency increment. A normalization is applied. A new analytical solution of the layer matrix equation is also given. This solution separates completely the treatment of the layers below and above the source.

Key words. Haskell matrices – Delta matrices – Numerical instabilities – Theoretical seismograms.

Introduction

Haskell layer matrix methods for the propagation of elastic waves in layered media have a wide range of application. However, numerical instabilities are a problem at high frequencies for phase velocities smaller than layer velocities. This problem requires improvements. Another problem is the large amount of computer time required for these methods. The Haskell layer matrix methods are an essential part of the reflectivity method for the computation of theoretical seismograms. Fuchs (1968) and Fuchs and Müller (1971) have developed this method. Dunkin (1965) and Watson (1970) have contributed to improvements in accuracy and speed of the Haskell layer matrix methods. Kind (1978) has published a computer program which was faster than earlier versions. An error in that program for the case of transmission was corrected by Baumgardt (1980). Abo-Zena (1979) has reformulated the layer matrix multiplication, resulting in improved computational accuracy. Kennett and Kerry (1979) and Woodhouse (1981) have developed different formulations of the buried source problem. Besides the reflectivity method, layer matrix methods are also used in mode summation methods for the computation of theoretical seismograms (Harvey, 1981).

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The Layered Halfspace with a Buried Source

We consider $P-SV$ plane wave propagation in a layered halfspace with a free surface. The source, represented by a discontinuity of the displacement-stress vector, is buried in the medium, and we are interested in the surface displacements. A layer n is bounded above by the interface $n-1$ and below by the interface n. The displacement-stress vector T_n of the interface n is related to T_{n-1}, the corresponding vector of the interface $n-1$, by the relation $T_n = B_n \cdot T_{n-1}$, where B_n is the Haskell layer matrix of layer n. The displacement-stress vectors are 4×1 matrices, and the Haskell matrices are 4×4 matrices. For a stack of layers the Haskell matrix is simply the product of the individual Haskell layer matrices. The displacement-stress vector is continuous at each interface, except at the source interface m, where we have $T_m^+ = T_m^- + S$. The plus or minus sign denotes location of T just below or above the interface m. S describes the displacement-stress vector of the source. This results in $T_k = B \cdot S + B \cdot T_m^-$, where k indicates the lowermost boundary, and B is the product of all Haskell matrices below the source. T_m^- can now be carried to the free surface, leading to $T_m^- = A \cdot T_0$, where A is the product of the Haskell layer matrices above the source, and $T_0 = (u, w, 0, 0)$ is the displacement-stress vector of the free surface with zero stress components, and the radial and vertical displacements u and w. Now we have

$$T_k = B \cdot (A \cdot T_0 + S). \qquad (1)$$

This is the basic equation relating the displacement-stress vector at the free surface to that at the lowermost boundary and to that of the source. T must be expressed by the potential coefficients for up- and downgoing waves in the halfspace, because we want to set these coefficients for upgoing waves equal to zero. This means we want no source at infinity. We have $T_k = E_k \cdot K_k$, where K_k is the vector of the potential coefficients and E_k is a matrix relating these two vectors. The elements of E_k, of the Haskell matrices, and of the source vector S for some sources can be found in Harkrider (1964). Kind (1979) gave the elements of S for a dislocation source. For only downgoing waves we have $K = (K_1, K_1, K_2, K_2)$, where K_1 and K_2 are the potential coefficients for P and SV waves, respectively. Then we may write

$$\begin{pmatrix} K_1 \\ K_1 \\ K_2 \\ K_2 \end{pmatrix} = E_k^{-1} \cdot B \cdot \begin{pmatrix} W \\ X \\ Y \\ Z \end{pmatrix} \tag{2}$$

and

$$\begin{pmatrix} W \\ X \\ Y \\ Z \end{pmatrix} = A \cdot \begin{pmatrix} u \\ w \\ 0 \\ 0 \end{pmatrix} + S. \tag{3}$$

First we solve (2) for W and X. In order to do that we multiply (2) with the matrix F, defined by

$$F = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}.$$

Multiplication with F means subtraction of row 2 from row 1, and of row 4 from row 3. Using $P = F \cdot E_k^{-1} \cdot B$, we obtain

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = P \cdot \begin{pmatrix} W \\ X \\ Y \\ Z \end{pmatrix} \tag{4}$$

P is a two row, four column matrix. The solution of (4) for W and X is

$$\begin{aligned} &-(P_{11} \cdot P_{22} - P_{12} \cdot P_{21}) \cdot W \\ &\quad = Y(P_{13} \cdot P_{22} - P_{12} \cdot P_{23}) + Z(P_{14} \cdot P_{22} - P_{12} \cdot P_{24}) \\ &-(P_{11} \cdot P_{22} - P_{12} \cdot P_{21}) \cdot X \\ &\quad = Y(P_{11} \cdot P_{23} - P_{13} \cdot P_{21}) + Z(P_{11} \cdot P_{24} - P_{14} \cdot P_{21}). \end{aligned} \tag{5}$$

Now we recognize that the coefficients in (5) are subdeterminants of the P matrix (Dunkin, 1965). They form a delta matrix. A good explanation of delta matrices can be found in Zurmühl (1964). All possible 2×2 subdeterminants of the 2×4 P matrix form a 1×6 delta matrix R with the following convention for the indices:

$$R_{1t} = P \begin{pmatrix} 12 \\ lm \end{pmatrix} = P_{1l} \cdot P_{2m} - P_{1m} \cdot P_{2l}$$

where $t = 1, 2, 3, 4, 5, 6$ corresponds to the pair $lm = 12, 13, 14, 23, 24, 34$. With these definitions we obtain from (5)

$$\begin{aligned} R_{11} \cdot W &= R_{14} \cdot Y + R_{15} \cdot Z \\ -R_{11} \cdot X &= R_{12} \cdot Y + R_{13} \cdot Z. \end{aligned}$$

Rewriting this equation we obtain:

$$\begin{pmatrix} W \\ X \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \cdot \begin{pmatrix} Y \\ Z \end{pmatrix} = C \cdot \begin{pmatrix} Y \\ Z \end{pmatrix} \tag{6}$$

where the elements of C follow from the previous equation. The elements of the delta matrix R are also given by Harkrider (1970), for example. We have $R_{14} = R_{13}$, therefore $C_{22} = -C_{11}$. Since the delta matrix of a product matrix is equal to the product of the individual delta matrices, we can compute layer delta matrices and multiply them through the layers. This procedure is more stable numerically than the multiplication of Haskell matrices.

Now we need to solve Eq. (3). Rewriting (3) we have

$$\begin{aligned} \begin{pmatrix} W \\ X \end{pmatrix} - \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} &= A_1 \begin{pmatrix} u \\ w \end{pmatrix} \\ \begin{pmatrix} Y \\ Z \end{pmatrix} - \begin{pmatrix} S_3 \\ S_4 \end{pmatrix} &= A_2 \begin{pmatrix} u \\ w \end{pmatrix} \end{aligned} \tag{7}$$

with the column vector $S = (S_1, S_2, S_3, S_4)^T$ and

$$A_1 = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad A_2 = \begin{pmatrix} A_{31} & A_{32} \\ A_{41} & A_{42} \end{pmatrix}.$$

From (6) and (7) we obtain

$$(C \cdot A_2 - A_1) \begin{pmatrix} u \\ w \end{pmatrix} = \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} - C \begin{pmatrix} S_3 \\ S_4 \end{pmatrix}. \tag{8}$$

The solution of this equation leads directly to the desired surface displacements. Equation (8) is a new solution of Eq. (1), which separates the treatment of the layers below and above the source completely. The solution of (8) requires the computation of $\det(C \cdot A_2 - A_1)$. This determinant can be computed in two different ways. In the first way it may be obtained from the elements of C, A_2 and A_1. Secondly it may also be computed using delta matrices. Using the first method, the accuracy of (8) is not better than the accuracy of the solution by Kind (1978). The second method improves the accuracy considerably.

Computing the determinant in terms of delta matrices, we may define the 2×2 matrix

$$V \cdot A \cdot I = C \cdot A_2 - A_1 \tag{9}$$

with

$$V = \begin{pmatrix} -1 & 0 & C_{11} & C_{12} \\ 0 & -1 & C_{21} & C_{22} \end{pmatrix}.$$

A is still the Haskell product matrix of all layers above the source, and I is the two columns, four rows unit matrix, containing a one in the 11 and 22 element and zeros elsewhere. From (9) it follows that for the computation of $\det(C \cdot A_2 - A_1)$ we may multiply the reduced 5×1 delta matrix of I with the reduced 5×5 delta matrix of A for each layer above the source. Finally we must multiply the resulting 5×1 column vector with the 1×5 row vector of the reduced delta matrix derived from V. This procedure allows the direct computation of the desired determinant without using the squares of the elements of the Haskell matrix A. The solution of (8) still requires the computation of the first two rows of A. But there elements appear only linear in (8), no squares of these elements are present anymore.

Now we summarize what matrix multiplications are required for the solution of (8): Below the source we need the 1×5 row vector of the reduced product delta matrix to obtain C. Above the source we need the 5×1 column vector of the reduced product delta matrix to compute the determinant in (8). And secondly we need above the source the 4×2 column vectors of the product Haskell matrix. The elements of this matrix are still in (8). Above the source appear the Haskell elements as quotients with the determinant. The appearance of these quotients in (8) is very important for the normalization. Without normalization the accuracy of the solution of (8) is much reduced. The normalization below the source is simple. Some care is needed above the source, because delta and Haskell matrix elements must be normalized there with the same constant. Above the source a normalization is only possible if the determinant is computed from delta matrices. The additional computation of the required Haskell matrix elements causes no problems.

The solution of Eq. (1) given by Harkrider (1964) did not use delta matrices and was therefore only good for fast phase velocities. Harkrider (1970) used delta matrices but the stability of his second solution was also by far not sufficient. Kind (1978) and Wang and Herrmann (1980) found another solution, which was more stable but still not satisfying. But the solution of (8) is much more stable in connection with the method described in the next section.

A Second Improvement of the Problem of Numerical Instabilities

The Haskell matrices contain exponential factors with the argument

$$P = \pm i\omega/c \cdot r \cdot d$$

with circular frequency ω, imaginary unit i, layer thickness d, phase velocity c and the vertical wavenumber $\omega/c \cdot r$, where $r^2 = c^2/v^2 - 1$. The P- or S-velocity in the layer is v. For a phase velocity larger than the layer velocity P is imaginary and the exponential factor is only a phase term, causing no numerical problems. For a phase velocity smaller than the layer velocity, r is imaginary and P is real. In this case the absolute value of P increases with frequency, layer thickness and inverse phase velocity. The elements of the Haskell matrices use linear combinations of the exponential functions with positive and negative arguments P. The accuracy limit of a digital computer is soon reached for increasing P, when $\exp(P)$ and $\exp(-P)$ are added. The use of delta matrices avoids unnecessary operations with these exponentials, but it is in principle no solution to the problem. We also have no fundamental solution, but we suggest the following method, which is a practical solution:

It is known that the numerical problems may be reduced by subdividing thick layers. That means we may replace a thick layer, which causes problems, by two or more thinner layers and multiply their layer matrices in order to obtain the layer matrix of the thick layer. This procedure reduces the numerical problems. The layer thickness in the layer matrix is only contained in the argument P of the exponential term, where it appears as a product with the frequency. Therefore, a high frequency can be treated in exactly the same manner as a large layer thickness. That means we may obtain the layer matrix for a high frequency by computing layer matrices for lower frequencies and by multiplication of these lower frequency matrices. The sum of the lower frequencies must be equal to the high frequency, exactly as in the case of layer thicknesses. As a consequence we only have to compute a layer matrix for the frequency increment $\Delta\omega$, and then obtain layer matrices for frequencies which are multiples of the frequency increment, by matrix multiplication. This method is applicable for cases where layer matrices for an equidistant set of frequencies are required. This is for example the case for the computation of theoretical seismograms with the reflectivity method. The computation time is not increased with this method, if the computer program is set up carefully, even for large numbers of frequencies.

Now a few more details of the computation of layer product matrices should be discussed. We have three independent variables, which lead in the computer program to three loops. These three variables are the slowness (or the wavenumber), frequency and the layer index. Keeping in mind the method for the solution of the numerical problems just described, we find the following order of the loops over the three variables practical. First we keep the slowness fixed (this is the outermost loop), then we keep the layer index fixed (middle loop), and compute the layer matrices for a set of frequencies (innermost loop). This has also the advantage that frequency independent terms may easily be kept outside the innermost loop. A computer program has been written using the described methods. The program is applying the matrix multiplication in the frequency loop (for slow phase velocities) and has about the same speed as the complex version of the program published by Kind (1976), but its accuracy is much better. A speed factor of about two may be gained by keeping the frequency independent terms outside the innermost frequency loop (not possible for slow phase velocities with matrix multiplication in the frequency loop). Almost another factor of two may be gained on some computers, when the complex operations in the innermost loop are replaced by real and imaginary operations. In test runs we have checked the accuracy of the new method for frequencies up to 100 Hz, layer thicknesses up to 30 km and phase velocities smaller than 0.5 km/s and found for all these cases no indication of numerical instabilities on our Hewlett Packard 1000 minicomputer. The computations were carried out in single precision mode, where the HP 1000 has six decimal digits accuracy. We have attempted to run Abo Zena's (1979) case with a method similar to his method on a HP 1000 with no success. For the method suggested in this paper, his case was no problem at all for the same machine. It should be mentioned that Abo Zena's method is also considerably slower, because it does more matrix multiplications.

Conclusions

The most important result of this research is a practical solution for the problem of numerical instabilities. The new method computes high frequency layer matrices by a multiplication of lower frequency matrices. This implies that the method is most useful if layer matrices of a set of equidistant frequencies are required. The method also applies a normalization to avoid overflow. It was attempted to apply this method without the use of delta matrices. This attempt was not successful, so delta matrices must be used where the results can be expressed in terms of delta matrices. The above technique is not slower than earlier techniques and its accuracy is much better. It is a solution for practically all frequencies, layer thicknesses and phase velocities used in seismology. It is clearly more accurate and also faster than Abo Zena's (1979) method.

As a second result a new analytical solution was found for the case of a buried source in a layered medium. This solution improves the computational speed especially for deep sources. Applying these new methods and a number of other improvements in the programming technique, we developed new layer matrix programs, which are up to four times faster than our earlier versions and much more accurate.

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