Plane-wave reflection coefficients for anisotropic media: Practical implementation

Charles P. Ursenbach and Arnim B. Haase

ABSTRACT

A step-by-step procedure is described for calculating reflection coefficients between media of monoclinic or higher symmetry, which possess a mirror plane parallel to the horizontal reflecting plane between the two media. This is based on a theoretical description available in the literature, and attempts to make these valuable results available to a wider audience.

In general outline, one begins with an incident ray in the upper medium, specified by a polar and azimuthal angle. One form of the Christoffel equations can be used to obtain the slowness vector of the incident wave. Next, using another form of the Christoffel equations, and the constancy of the horizontal slowness components, one obtains a unique vertical slowness for each reflected and transmitted wave, six in all. Using the Christoffel equations once more, but in their original form, one can then obtain the polarization vectors of each reflected and transmitted wave. One then has sufficient information to construct impedance matrices, and these may be combined with matrix algebra to obtain two new matrices, one with all of the reflection coefficients and one with all of the transmission coefficients.

A key aspect of programming a non-trivial code such as this is testing. This paper includes benchmark numbers which can be used to begin rigorous testing of an implementation of the above theory.

INTRODUCTION

Schoenberg and Protázio (1992) have presented a method for computing reflection and transmission coefficients between two anisotropic media. The only restriction is that each medium must possess a mirror plane parallel to the interface. This excludes triclinic media, but allows monoclinic and all higher symmetries.

For a derivation of the theory we refer the reader to the paper of Schoenberg and Protázio (1992). This report is concerned with presenting a straightforward, step-by-step description of how the theory can be implemented in a computational setting, and then presenting a few benchmark tests that are useful in testing the resulting program.

THEORY

To begin with we review the notation of the Christoffel matrix and equations. The theoretical development then begins by obtaining the slowness vector of an incident wave of specified type and angle. Next we will obtain slowness and polarization vectors of the reflected and transmitted waves, each in their own medium. Following this we construct two 3 × 3 “impedance” matrices for each medium. Finally we will combine all four matrices to yield reflection and transmission coefficients at the interface for a given ray parameter or angle of incidence, analogous to the Zoeppritz coefficients for isotropic media.

Christoffel matrix and Christoffel equations

Various conventions have ascribed different meanings to the term 'Christoffel matrix'. We will denote its generic component as

$$\Gamma_{ik} = \sum_{jl} c_{ijkl} s_j s_l \;, \tag{1}$$

where c_{ijkl} is a component of the fourth-order elastic tensor for a single homogeneous medium, and s_i is a component of the slowness vector of a plane wave within that medium. As needed we will append the superscripts U and L to refer to the upper and lower media, respectively (e.g. c^U_{ijkl} , s^L_i , etc.).

It is common to take advantage of the symmetries of an elastic tensor and to notationally compress the 3 × 3 × 3 × 3 tensor into a 6 × 6 matrix, with elements c_{ij}. In this case the elements of the monoclinic Christoffel matrix are written as [compare with the expression following equation 27 of Schoenberg and Protázio, (1992)]

$$\begin{aligned}
\Gamma_{11} &= c_{11}s_1^2 + c_{66}s_2^2 + c_{55}s_3^2 + 2c_{16}s_1s_2 \\
\Gamma_{22} &= c_{66}s_1^2 + c_{22}s_2^2 + c_{44}s_3^2 + 2c_{26}s_1s_2 \\
\Gamma_{33} &= c_{55}s_1^2 + c_{44}s_2^2 + c_{33}s_3^2 + 2c_{45}s_1s_2 \\
\Gamma_{12} &= \Gamma_{21} = c_{16}s_1^2 + c_{26}s_2^2 + c_{45}s_3^2 + \left(c_{12} + c_{66}\right)s_1s_2 \\
\Gamma_{13} &= \Gamma_{31} = \left(c_{13} + c_{55}\right)s_1s_3 + \left(c_{36} + c_{45}\right)s_2s_3 \\
\Gamma_{23} &= \Gamma_{32} = \left(c_{36} + c_{45}\right)s_1s_3 + \left(c_{23} + c_{44}\right)s_2s_3
\end{aligned} \;. \tag{2}$$

In the orthotropic case, these equations simplify to

$$\begin{aligned}
\Gamma_{11} &= c_{11}s_1^2 + c_{66}s_2^2 + c_{55}s_3^2 \\
\Gamma_{22} &= c_{66}s_1^2 + c_{22}s_2^2 + c_{44}s_3^2 \\
\Gamma_{33} &= c_{55}s_1^2 + c_{44}s_2^2 + c_{33}s_3^2 \\
\Gamma_{12} &= \Gamma_{21} = \left(c_{12} + c_{66}\right)s_1s_2 \\
\Gamma_{13} &= \Gamma_{31} = \left(c_{13} + c_{55}\right)s_1s_3 \\
\Gamma_{23} &= \Gamma_{32} = \left(c_{23} + c_{44}\right)s_2s_3
\end{aligned} \;, \tag{3}$$

but note that if the axes of the orthotropic medium are rotated azimuthally about the vertical coordinate axis, then the resulting Christoffel matrix will have the monoclinic form, as in equation 2. [Elastic constants for a medium which has been rotated relative to the crystallographic coordinate system can be obtained using the Bond transformation (Winterstein, 1990)]. Other Christoffel matrices of interest are for the HTI case,

$$\begin{aligned}
\Gamma_{11} &= c_{11}s_1^2 + c_{66}\left(s_2^2 + s_3^2\right) \\
\Gamma_{22} &= c_{66}s_1^2 + c_{33}s_2^2 + c_{44}s_3^2 \\
\Gamma_{33} &= c_{66}s_1^2 + c_{44}s_2^2 + c_{33}s_3^2 \\
\Gamma_{12} &= \Gamma_{21} = \left(c_{13} + c_{66}\right)s_1s_2 \\
\Gamma_{13} &= \Gamma_{31} = \left(c_{13} + c_{66}\right)s_1s_3 \\
\Gamma_{23} &= \Gamma_{32} = \left(c_{33} - c_{44}\right)s_2s_3
\end{aligned}, \tag{4}$$

the VTI case,

$$\begin{aligned}
\Gamma_{11} &= c_{11}s_1^2 + c_{66}s_2^2 + c_{44}s_3^2 \\
\Gamma_{22} &= c_{66}s_1^2 + c_{11}s_2^2 + c_{44}s_3^2 \\
\Gamma_{33} &= c_{44}\left(s_1^2 + s_2^2\right) + c_{33}s_3^2 \\
\Gamma_{12} &= \Gamma_{21} = \left(c_{11} - c_{66}\right)s_1s_2 \\
\Gamma_{13} &= \Gamma_{31} = \left(c_{13} + c_{44}\right)s_1s_3 \\
\Gamma_{23} &= \Gamma_{32} = \left(c_{13} + c_{44}\right)s_2s_3
\end{aligned}, \tag{5}$$

and the isotropic case,

$$\begin{aligned}
\Gamma_{11} &= c_{11}s_1^2 + c_{44}\left(s_2^2 + s_3^2\right) = \left(\lambda + 2\mu\right)s_1^2 + \mu\left(s_2^2 + s_3^2\right) \\
\Gamma_{22} &= c_{44}s_1^2 + c_{11}s_2^2 + c_{44}s_3^2 = \left(\lambda + 2\mu\right)s_2^2 + \mu\left(s_1^2 + s_3^2\right) \\
\Gamma_{33} &= c_{44}\left(s_1^2 + s_2^2\right) + c_{11}s_3^2 = \left(\lambda + 2\mu\right)s_3^2 + \mu\left(s_1^2 + s_2^2\right) \\
\Gamma_{12} &= \Gamma_{21} = \left(c_{12} + c_{44}\right)s_1s_2 = \left(\lambda + \mu\right)s_1s_2 \\
\Gamma_{13} &= \Gamma_{31} = \left(c_{12} + c_{44}\right)s_1s_3 = \left(\lambda + \mu\right)s_1s_3 \\
\Gamma_{23} &= \Gamma_{32} = \left(c_{12} + c_{44}\right)s_2s_3 = \left(\lambda + \mu\right)s_2s_3
\end{aligned}. \tag{6}$$

The Christoffel equations arise naturally from assuming a plane-wave solution to the anisotropic wave equation. They can be expressed in terms of the Christoffel matrix as [compare with equation 27 of Schoenberg and Protázio, (1992)]

$$\left(\underline{\underline{\Gamma}} - \rho\underline{\underline{I}}\right)\underline{u} = 0, \tag{7}$$

where ρ is the density of the medium, and $\underline{u}$ is the polarization vector of the wave.

Slowness vector of the incident wave

We assume that an incident wave is specified. This requires specification of the wave as compressional, shear vertical, or shear horizontal. (Although the meaning of these terms becomes blurred for anisotropic media, we will assume that the anisotropy is sufficiently weak that the terms are still useful.) It also requires knowledge of its polar angle (θ) relative to the interface normal, and its azimuthal angle (ϕ) relative to some specified *x*-axis. The *x*- and *y*-axes are usually defined to lie along the symmetry axes of at least one of the two media.

Assuming the incident wave originates in the upper medium, we begin by writing the Christoffel equations for the upper medium. However in this instance we multiply them by V^2/ρ, so they are of the form

$$\left(\underline{\underline{\Lambda}}^U - V^2 \underline{\underline{I}}\right)\underline{u} = 0\,, \tag{8}$$

where

$$\begin{gathered}\Lambda_{11}^U = a_{11}^U n_1^2 + a_{66}^U n_2^2 + a_{55}^U n_3^2 + 2a_{16}^U n_1 n_2 \\ \text{etc.}\end{gathered}\,. \tag{9}$$

and where $a_{ij} = c_{ij}/\rho$ and $n_i = Vs_i$. Thus $\underline{n} = \left(\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta\right)$ is a unit vector parallel to the wavefront normal, and is known for the incident wave, as are the $\{a_{ij}\}$.

Nontrivial solutions to equation 8 exist only under the condition

$$\left|\underline{\underline{\Lambda}}^U - V^2 \underline{\underline{I}}\right| = 0\,, \tag{10}$$

which is a cubic equation in V^2 (also called bicubic in *V*). The three solutions of equation 10 are eigenvalues of equation 8, and provide us with velocities of P-waves and two different S-waves moving through the upper medium in the direction $\underline{n}$. Following Schoenberg and Protázio we will denote these velocities V_P, V_S and V_T. Physically, these should always be positive, real numbers (so that the eigenvalues, V^2, should also be positive and real). The three corresponding slowness vectors then are

$$\underline{s}_P = \left\{\frac{n_1}{V_P}, \frac{n_2}{V_P}, \frac{n_3}{V_P}\right\}, \tag{11}$$

$$\underline{s}_S = \left\{\frac{n_1}{V_S}, \frac{n_2}{V_S}, \frac{n_3}{V_S}\right\}, \tag{12}$$

$$\underline{s}_T = \left\{\frac{n_1}{V_T}, \frac{n_2}{V_T}, \frac{n_3}{V_T}\right\}. \tag{13}$$

For seismic applications we will assume the incident wave to be compressional, and will thus assume that the incident wave slowness vector is given by equation 11.

Slowness vectors of reflected and transmitted waves

We will require the slowness vectors for all reflected and transmitted waves. The horizontal components are already known, as they will be identical to those of the incident wave. Thus if the incident wave is a P-wave, for instance, then the horizontal components will always be given by n_1/V_P and n_2/V_P. To obtain the vertical slowness for reflected and transmitted waves (which is n_3/V_P for the incident wave) we will use two Christoffel equations of the form of equation 7, one for the upper medium and one for the lower medium. These will only possess solutions again when their determinants are equal to zero, i.e.

$$\left|\underline{\underline{\Gamma}}^U - \rho^U \underline{\underline{I}}\right| = 0 , \tag{14}$$

$$\left|\underline{\underline{\Gamma}}^L - \rho^L \underline{\underline{I}}\right| = 0 . \tag{15}$$

The only unknown quantity in each of these equations is now s_3, and each equation forms a bicubic equation in s_3. (This is because of the requirement of a mirror plane of symmetry in each medium. Otherwise they would generally form sextic equations.) Equation 14 yields three solutions for s_3^2. If a given reflected or transmitted wave is homogeneous (pre-critical), then its corresponding s_3^2 value will be positive, and s_3 may be positive or negative. The *negative* square roots of these values give the vertical slownesses for the P, S and T *reflected* waves. (As a check, the vertical slowness of the reflected P-wave should equal $-n_3/V_P$, by symmetry.) Similarly equation 15 yields three other solutions for s_3^2, and the *positive* square roots of these give the vertical slownesses for the P, S and T *transmitted* waves. This employs the convention that downgoing is positive and upgoing is negative.

Having belaboured this point, we now emphasize that the expressions of Schoenberg and Protázio (1992) account for the signs, so one may always apply the positive value of s_3 .

These vertical slownesses, combined with the horizontal slownesses already known, thus yield the six slowness vectors of the reflected and transmitted waves, for the given incident P-wave.

Polarization vectors of reflected and transmitted waves

We can now revisit equation 7 and solve it for $\underline{u}$. We will do this six times, once for each different value of s_3. For the three reflected waves we will use

$$\left(\underline{\underline{\Gamma}}^U - \rho^U \underline{\underline{I}}\right)\underline{u} = 0 , \tag{16}$$

and for the three transmitted waves we will use

$$\left(\underline{\underline{\Gamma}}^L - \rho^L \underline{\underline{I}}\right)\underline{u} = 0 \ . \tag{17}$$

Because these are homogeneous systems of equations, we can only solve in terms of a parameter. For instance, we can use two of the three equations to obtain expressions of the form

$$\begin{aligned} u_1 &= a u_3 \\ u_2 &= b u_3. \end{aligned} \tag{18}$$

The third equation will add no further information, and one generally assumes normalization at this point,

$$1 = u_1^2 + u_2^2 + u_3^2 , \tag{19}$$

so that

$$u_3 = 1 - a^2 - b^2 \tag{20}$$

and u_1 and u_2 can then be obtained from equation 18. This occurs without complication for homogeneous waves, for which all components of $\underline{u}$ are real. For an inhomogeneous wave though at least one component of $\underline{u}$ is imaginary. Conventionally when normalizing complex eigenvectors one employs the relation

$$1 = |u_1|^2 + |u_2|^2 + |u_3|^2 . \tag{21}$$

In this case, however, this is wrong, and one should use equation 19 instead, even for complex eigenvectors, in order for the expressions of Schoenberg and Protázio (1992) to work correctly.

Results so far: Slowness and polarization vectors for each medium

Collecting results obtained thus far, we have slowness and polarization vectors for reflected waves in the upper medium, and for transmitted waves in the lower medium. Let us explicitly give the notation, as it will help keep things straight in the next section:

Upper medium:

$$\underline{s}_P^r = \left\{ s_1, s_2, s_{P,3}^r \right\}, \quad \underline{u}_P^r = \left\{ u_{P,1}^r, u_{P,2}^r, u_{P,3}^r \right\} \tag{21}$$

$$\underline{s}_S^r = \left\{ s_1, s_2, s_{S,3}^r \right\}, \quad \underline{u}_S^r = \left\{ u_{S,1}^r, u_{S,2}^r, u_{S,3}^r \right\} \tag{22}$$

$$\underline{s}_T^r = \left\{ s_1, s_2, s_{T,3}^r \right\}, \quad \underline{u}_T^r = \left\{ u_{T,1}^r, u_{T,2}^r, u_{T,3}^r \right\} \tag{23}$$

Lower medium:

$$\underline{s}_P^t = \left\{ s_1, s_2, s_{P,3}^t \right\}, \quad \underline{u}_P^t = \left\{ u_{P,1}^t, u_{P,2}^t, u_{P,3}^t \right\} \tag{24}$$

$$\underline{s}_S^t = \left\{ s_1, s_2, s_{S,3}^t \right\}, \quad \underline{u}_S^t = \left\{ u_{S,1}^t, u_{S,2}^t, u_{S,3}^t \right\} \tag{25}$$

$$\underline{s}_T^t = \left\{ s_1, s_2, s_{T,3}^t \right\}, \quad \underline{u}_T^t = \left\{ u_{T,1}^t, u_{T,2}^t, u_{T,3}^t \right\} \tag{26}$$

The upper subscripts refer to reflected (r) or transmitted (t), and the lower subscripts refer to the wave type (P, S, or T) and to the Cartesian direction (1, 2, or 3).

Impedance matrices

Schoenberg and Protázio (1992) then give the reflection and transmission coefficients in terms of 3-by-3 **X** and **Y** matrices. Using the notation of equations 21-26, we obtain [compare with equation 31 of Schoenberg and Protázio, (1992)]

$$\mathbf{X}^U = \begin{bmatrix} u_{P,1}^r & u_{S,1}^r & u_{T,1}^r \\ u_{P,2}^r & u_{S,2}^r & u_{T,2}^r \\ \begin{array}{l} -(c_{13}u_{P,1}^r + c_{36}u_{P,2}^r)s_1 \\ -(c_{23}u_{P,2}^r + c_{36}u_{P,1}^r)s_2 \\ -c_{33}u_{P,3}^r s_{P,3} \end{array} & \begin{array}{l} -(c_{13}u_{S,1}^r + c_{36}u_{S,2}^r)s_1 \\ -(c_{23}u_{S,2}^r + c_{36}u_{S,1}^r)s_2 \\ -c_{33}u_{S,3}^r s_{S,3} \end{array} & \begin{array}{l} -(c_{13}u_{T,1}^r + c_{36}u_{T,2}^r)s_1 \\ -(c_{23}u_{T,2}^r + c_{36}u_{T,1}^r)s_2 \\ -c_{33}u_{T,3}^r s_{T,3} \end{array} \end{bmatrix}, \tag{27}$$

$$\mathbf{Y}^U = \begin{bmatrix} -(c_{55}s_1 + c_{45}s_2)u^r_{P,3} & -(c_{55}s_1 + c_{45}s_2)u^r_{S,3} & -(c_{55}s_1 + c_{45}s_2)u^r_{T,3} \\ -(c_{55}u^r_{P,1} + c_{45}u^r_{P,2})s^r_{P,3} & -(c_{55}u^r_{S,1} + c_{45}u^r_{S,2})s^r_{S,3} & -(c_{55}u^r_{T,1} + c_{45}u^r_{T,2})s^r_{T,3} \\ -(c_{45}s_1 + c_{44}s_2)u^r_{P,3} & -(c_{45}s_1 + c_{44}s_2)u^r_{S,3} & -(c_{45}s_1 + c_{44}s_2)u^r_{T,3} \\ -(c_{45}u^r_{P,1} + c_{44}u^r_{P,2})s^r_{P,3} & -(c_{45}u^r_{S,1} + c_{44}u^r_{S,2})s^r_{S,3} & -(c_{45}u^r_{T,1} + c_{44}u^r_{T,2})s^r_{T,3} \\ u^r_{P,3} & u^r_{S,3} & u^r_{T,3} \end{bmatrix}.$$

(28)

For the lower layer one obtains $\mathbf{X}^L$ and $\mathbf{Y}^L$ from expressions identical to equations 27 and 28, but with the superscript *r* replaced by *t*.

Reflection and transmission coefficients

The **X** and **Y** matrices encode all necessary information about each layer. They are combined to yield reflection and transmission coefficients in the following manner [compare with equation 10 of Schoenberg and Protázio, (1992)]:

$$\mathbf{D} = \left(\mathbf{X}^U\right)^{-1}\mathbf{X}^L + \left(\mathbf{Y}^U\right)^{-1}\mathbf{Y}^L, \tag{29}$$

$$\mathbf{R} = \left[\left(\mathbf{X}^U\right)^{-1}\mathbf{X}^L - \left(\mathbf{Y}^U\right)^{-1}\mathbf{Y}^L\right]\mathbf{D}^{-1}, \tag{30}$$

$$\mathbf{T} = 2\mathbf{D}^{-1}, \tag{31}$$

where matrices **R** and **T** are interpreted as containing reflection and transmission coefficients as follows [compare with equation 10 of Schoenberg and Protázio, (1992), which is transposed relative to these expressions]:

$$\mathbf{R} = \begin{bmatrix} R_{PP} & R_{SP} & R_{TP} \\ R_{PS} & R_{SS} & R_{TS} \\ R_{PT} & R_{ST} & R_{TT} \end{bmatrix}, \tag{32}$$

$$\mathbf{T} = \begin{bmatrix} T_{PP} & T_{SP} & T_{TP} \\ T_{PS} & T_{SS} & T_{TS} \\ T_{PT} & T_{ST} & T_{TT} \end{bmatrix}. \tag{33}$$

IMPLEMENTATION AND TESTING

The above method has been implemented in MATLAB and is included in the software distribution to sponsors for the 2007 software release. There is no extant set of benchmarks for testing orthorhombic plane-wave reflection coefficient programs, but the code has been tested as described next.

Comparison has been made with values extracted from Figure 4 of Ruger (1997) which claims to contain exact results for plane waves in an isotropic medium reflecting off of an interface with an HTI medium. The extracted values (which we could only estimate with two-digit accuracy) are shown in the third column of Table 1. Results from our code are given in the fourth column. Our results appear to agree with Figure 4 of Ruger (1997). Comparison can only be made with the results for azimuthal angles of 30° and 60° and non-zero offset, because the method above is numerically unstable for $\theta = 0°$ and for $\phi = 0°$ and 90°. It is possible in this case that the 3-by-3 matrix formulation reduces to 2-by-2 matrix expressions. (See for instance pages 133-136 of Schoenberg and Protázio.) In these cases, values of ϕ close to 0° and 90° and of θ close to 0° have been employed and again appear to agree with Ruger's results.

Table 1. Values of $R_{PP}(\theta)$ as given by Ruger (1997) compared with results obtained in this study.

θ	ϕ	Fig. 4 of Ruger (1997)	Present study
0°	-	0.066	0.06635615 (θ, ϕ) =(1°, 60°) 0.06637131 (1°, 30°) 0.06636817 (0.8°, 30°)
40°	0°	0.096	0.09589535 (40°, <0.000001°)
40°	30°	0.087	0.08708026

40°	60°	0.072	0.07165368
40°	90°	0.065	0.06511655 (40°,90.1°)

Some aspects of this program's capabilities that are *not* tested by the results of Table 1 include

- full orthorhombic symmetry
- an anisotropic overburden
- non-alignment of upper and lower medium symmetry axes
- behavior beyond the critical angle

Further testing of this program might be accomplished using results from Rüger and Tsvankin (1997) and from Vavryčuk and Pšenčik (1998).

CONCLUSIONS

The original work of Schoenberg and Protázio (1992) provides a derivation of expressions useful for calculating reflection and transmission coefficients between two media of monoclinic or higher symmetry, as long as both media contain mirror planes of symmetry parallel to the interface. However, it may not be obvious, particularly to the uninitiated, how such expressions are to be implemented in a computer program. This report repackages the results of Schoenberg and Protázio (1992) in a way that is designed to make their work more accessible for a computer programmer. A set of benchmark results have also been provided which may be useful in testing programs based on this method.

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