A comparison of finite difference analogs for hyperbolic equations in inhomogeneous media

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ABSTRACT

In an infinite halfspace with constant media, scalar wave equations may be written including one for acoustic wave propagation (pressure wave propagation in fluids) and another for S_H-wave potential propagation. Both of these scalar wave equations will be considered here in a radially symmetric medium with the possibility that parameters related to both problems may vary with depth. This is done such that the different effects of discontinuities with depth of the media parameters may be investigated in the context of the boundary conditions required to be introduced. Once these have been determined, finite different analogues for the two cases are constructed. The simplest of these cases is to consider incidence at the halfspace boundary with the upper halfspace assumed to be a vacuum as was considered by Aki and Richards who presented solutions in the form of Sommerfeld integrals. For the problem types being investigated here, stress continuity conditions for a horizontal boundary within the two media types will be addressed.

What has often been noticed in the literature is that a scalar wave equation associated with elastodynamic wave propagation in an isotropic homogeneous medium has its parameters modified, without any mathematical justification, to be spatially variable and the resulting equation employed to model elastodynamic (compressional) $P-$wave propagation using methods such as finite difference modeling. Liberties appear to be taken regarding continuity conditions at discontinuities of media parameters (interfaces). This is not to say that reasonable looking numerical results cannot be obtained, but the nature of these equations is questioned.

INTRODUCTION

The compressional (P) scalar potential wave equation as well as the acoustic (pressure) wave equation and S_H-wave potential equation for an isotropic homogeneous halfspace all have the similar form,

$$\rho v^2\nabla^2\phi(\mathbf{r},t)-\rho\frac{\partial^2\phi(\mathbf{r},t)}{\partial t^2}=\partial(\mathbf{r}-\mathbf{r}_0)f(t) \tag{1}$$

following Aki and Richards (1980) where $\mathbf{r}$ is a $3D$ position vector, t is time, v is the propagation velocity, and the potential ϕ can be a scalar $P-$wave potential, the acoustic pressure $P(\mathbf{r},t)$ related to wave propagation in fluids or $\psi(\mathbf{r},t)$ which is the scalar potential related to the S_H displacement, $\mathbf{v}(\mathbf{r},t)$. The polarization vector associated with this displacement type is normal to the incident plane and is expressed in terms of $\psi(\mathbf{r},t)$ in a Cartesian system as $\mathbf{v}=(0,v,0)=\nabla\psi(\mathbf{r},t)$. There is a difference between the above two potential equations, which will be investigated here. The S_H potential equation is obtained by introducing the quantity $\mathbf{v} = \nabla \times (0,0,\psi)$ into the elastodynamic equation with spatially dependent Lamé coefficients and density with the result given in equation (3).

As the intent of this report is to address certain finite difference analogue matters related to discontinuities in the parameters $(\alpha \text{ and } \rho)$ in equation (1), it may be useful to refer to a relevant article in the literature. In Shuster's freely available $P-S_V$ finite difference computer code for a $2D$ plane layered isotropic medium, the continuity equations involving particle displacements and stresses at the interfaces between two elastic media are explicitly introduced. There are numerous articles where establishing the continuity conditions is done in an explicit manner. The basis for the implicit establishment of continuity conditions is established using effective media parameters or harmonic averages of the media parameters.

The use of effective media parameters (harmonic averages) has been employed by numerous authors in finite difference modeling to account for continuity conditions at media parameter discontinuities (see for example, Boore, 1972; Schoenberg and Muir, 1989, Levander, 1988, Moczo, 1989, Zahradnik et al., 1993, Graves, 1996). It was shown by Zahradnik et al. (1993) that the effective media parameters (harmonic averages) provide a more accurate representation of the actual parameters in the region near media interfaces by appropriately satisfying the traction continuity condition across the interface. While the shear and bulk moduli employ harmonic averaging, arithmetic averaging of the density is most commonly used. It should be noted in the above that the interfaces lie along horizontal grid lines. The progression to interfaces specified along vertical grid lines follows. It appears to still be point of discussion as to how to properly deal with arbitrary media boundaries that do not lie along either vertical or horizontal grid lines. Anecdotally, results may apparently be improved to some extent by using 9 or 25 grid points centered on the grid point near which the boundary is at some angle with the finite difference grid. This is not usually a preferred option, being computationally intensive in space and run time.

THEORY

Consider a 2.5 dimensional radially symmetric coordinate system, (r,z), in a halfspace $z > 0$. An explosive point source is located at $\mathbf{r} = \mathbf{r}_0$, the acoustic pressure equation (1) has the form for the acoustic wave equation with variable density may be written as

$$K\nabla\left[\frac{1}{\rho(\mathbf{r})}\nabla P(\mathbf{r},t)\right] - \frac{\partial^2 P(\mathbf{r},t)}{\partial t^2} = \delta(\mathbf{r}-\mathbf{r}_0)\, f(t) \qquad (2)$$

where K is the rigidity, which in the most general case could have a time dependence, but is not spatially dependent. The density, $\rho(\mathbf{r})$, is assumed to be spatially dependent such that spatial variations of $\rho(\mathbf{r})$ specify the heterogeneities of the material properties of the medium.

Alternately, the S_H potential wave equation with a spatially variable Lamé's coefficient, $\mu(\mathbf{r})$, and density, $\rho(\mathbf{r})$, is given by

$$\nabla\left[\mu(\mathbf{r})\nabla\psi(\mathbf{r},t)\right]-\rho(\mathbf{r})\frac{\partial^2\psi(\mathbf{r},t)}{\partial t^2}=\delta(\mathbf{r}-\mathbf{r}_0)f(t) \tag{3}$$

The equations (2) and (3) fully specify an initial value problem if the values of $\phi|_{t=0}$ and $\partial\phi/\partial t|_{t=0}$ are indicated, usually as $\phi|_{t=0}=\partial\phi/\partial t|_{t=0}=0$, where ϕ may be either the acoustic pressure, $P(\mathbf{r},t)$ or the shear wave potential, $\psi(\mathbf{r},t)$.

The reason for writing equations (2) and (3) in the forms above rather than as something similar to equation (1) is so that if they are to be employed in modeling using finite difference methods, boundary conditions, at least at horizontal and vertical grid planes, are satisfied implicitly. The rationale for this is to satisfy the physical laws used in their derivation. Discussions of this topic for the S_H problem appear in a number of works such as Alterman and Karal (1968), Boore (1972), Kelly et al. (1976), Kummer and Behle (1982), Kummer et al. (1987), Moczo (1989) and Zahradnik et al. (1993), among others. Acoustic wave propagation is also addressed in many works. However, the paper by Sochacki et al. (1991) contains a more than acceptable treatment and cites a variety of related works.

It will now be convenient to return to equation (1) and as the velocity has been assumed spatially invariant, a finite Hankel transform (Appendix A and Mikhailenko, 1985,1988) will be applied to remove the radial component for the time being, leaving a problem in depth and time as follows

$$-\zeta_n^2\rho\alpha^2\phi+\rho\alpha^2\frac{\partial^2\phi}{\partial z^2}-\rho\frac{\partial^2\phi}{\partial t^2}=\frac{\delta(z-z_0)}{2\pi}f(t) \tag{4}$$

This form of the scalar wave equation appears in the geophysical literature on a regular basis, often with the assumption that the elastic parameters (velocity) are spatially dependent. As equations (2) and (3) appear in a manner that adheres to the physical principles from which they were derived, the question is what set of physical conditions were initially used to arrive at equation (4) having the form

$$-\zeta_n^2\rho(z)\alpha^2(z)\phi+\rho(z)\alpha^2(z)\frac{\partial^2\phi}{\partial z^2}-\rho(z)\frac{\partial^2\phi}{\partial t^2}=\frac{\delta(z-z_0)}{2\pi}f(t) \tag{5}$$

In addition, what form of finite difference analogue with respect to the z (depth) coordinate would adequately satisfy these physical principles? This is apparently a set of two coupled questions in two unknown answers. The most direct route (letting $\rho\alpha^2=\zeta$) would be to use

$$\zeta(z)\frac{\partial^2\phi}{\partial z^2} \approx \zeta_n\left(\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{(\Delta z)^2}\right) \tag{6.a}$$

or possibility

$$\zeta(z)\frac{\partial^2\phi}{\partial z^2} \approx \left(\frac{\zeta_{n+1/2}+\zeta_{n-1/2}}{2}\right)\left(\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{(\Delta z)^2}\right) \tag{6.b}$$

or even

$$\zeta(z)\frac{\partial^2\phi}{\partial z^2} \approx \left(\frac{\bar{\zeta}_{n+1/2}+\bar{\zeta}_{n-1/2}}{2}\right)\left(\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{(\Delta z)^2}\right). \tag{6.c}$$

where $\left[\zeta_{n+1/2}(z)+\zeta_{n-1/2}(z)\right]/2=\left[\zeta_{n+1}(z)+2\zeta_n(z)+\zeta_{n-1}(z)\right]/4$ and the harmonic average quantities, $\bar{\zeta}_{n\pm1/2}(z)$, are defined below.

Another possibility might be to emulate equations (2) and (3), using less than mathematically rigorous methods, to initially obtain

$$\bar{\zeta}(z)\frac{\partial^2\phi}{\partial z^2} \approx \frac{\bar{\zeta}(z)}{\Delta z}\left[\left(\frac{\phi_{n+1}-\phi_n}{\Delta z}\right)-\left(\frac{\phi_n-\phi_{n-1}}{\Delta z}\right)\right] \tag{7}$$

where $\bar{\zeta}(z)$ is the harmonic average of $\zeta(z)$. An analogue for the quantity $\bar{\zeta}(z)$ may be introduced into equation (7) resulting in

$$\begin{aligned}\bar{\zeta}(z)\frac{\partial^2\phi}{\partial z^2} &\approx \frac{1}{\Delta z}\left[\left(\frac{\phi_{n+1}-\phi_n}{\Delta z}\right)\bar{\zeta}_{n+1/2}(z)-\left(\frac{\phi_n-\phi_{n-1}}{\Delta z}\right)\bar{\zeta}_{n-1/2}(z)\right] \\ &\approx \frac{\bar{\zeta}_{n+1/2}(z)\phi_{n+1}-\left(\bar{\zeta}_{n+1/2}(z)+\bar{\zeta}_{n-1/2}(z)\right)\phi_n+\bar{\zeta}_{n-1/2}(z)\phi_{n-1}}{(\Delta z)^2}\end{aligned} \tag{8}$$

where the harmonic average terms $\bar{\zeta}_{n\pm1/2}(z)$ are defined as

$$\bar{\zeta}_{n+1/2}(z) \approx \left[\frac{1}{2}\left(\frac{1}{\zeta_{n+1}}+\frac{1}{\zeta_n}\right)\right]^{-1} = \frac{2\zeta_{n+1}\zeta_n}{\zeta_{n+1}+\zeta_n} = \chi_{n+1} \tag{9}$$

and

$$\bar{\zeta}_{n-1/2}(z) \approx \left[\frac{1}{2}\left(\frac{1}{\zeta_n}+\frac{1}{\zeta_{n-1}}\right)\right]^{-1} = \frac{2\zeta_n\zeta_{n-1}}{\zeta_n+\zeta_{n-1}} = \chi_{n-1} \tag{10}$$

respectively. This manner of obtaining a finite difference analog for the differential term in z, as shown above, results in

$$\frac{1}{\Delta z}\left[\left(\frac{\phi_{n+1}-\phi_n}{\Delta z}\right)\chi_{n+1}-\left(\frac{\phi_n-\phi_{n-1}}{\Delta z}\right)\chi_n\right]=\frac{\chi_{n+1}\phi_{n+1}-\left(\chi_{n+1}+\chi_n\right)\phi_n+\chi_n\phi_{n-1}}{\left(\Delta z\right)^2}. \quad (11)$$

It remains to be determined what this means. Assume that $\phi = Ae^{i\omega t - i\omega\xi z}$ with $\xi = \left(\alpha^{-2} - p^2\right)^{1/2}$, $p -$ horizontal component of the slowness vector, and that in a manner similar at least to the S_H that at some horizontal plane where the velocity is discontinuous that the condition ("$-$" just above discontinuity and "+" just below discontinuity)

$$\left[\rho\alpha^2(z)\frac{\partial\phi}{\partial z}\right]_- = \left[\rho\alpha^2(z)\frac{\partial\phi}{\partial z}\right]_+. \quad (12)$$

so that

$$\rho\alpha^2(z_-)\xi_- A_- = \rho\alpha^2(z_+)\xi_+ A_+ \quad \to \quad \rho\alpha(z_-)\cos\theta_- A_- = \rho\alpha(z_+)\cos\theta_+ A_+. \quad (13)$$

as using the standard definition of p, then $\cos\theta = \left(1-\alpha^2 p^2\right)^{1/2}$. Upon reviewing the text of Aki and Richards (1980) this may be taken to be some modified form of $P-$wave normal stress, yielding an expression very similar to that resulting when considering the S_H problem (Zhahradnik et al., 1993)

$$\rho(z_-)\alpha(z_-)\cos\theta_- A_- = \rho(z_+)\alpha(z_+)\cos\theta_+ A_+. \quad (14)$$

This formula, as is shown in the next section, would produce results that are not what would be expected for $P-$wave propagation.

In the case of a plane wave incident from the $(-)$ medium, $A_- = 1-R$ and $A_+ = T$, where R and T are the S_H (plane wave) reflection and transmission coefficients. The additional equation required to solve for R and T is the continuity of the scalar potential given as $1+R=T$. For comparison purposes (Brekhovskikh, 1980), the acoustic pressure wave is afforded a similar treatment as above so that

$$\left[\frac{1}{\rho(z)}\frac{\partial\phi}{\partial z}\right]_- A_- = \left[\frac{1}{\rho(z)}\frac{\partial\phi}{\partial z}\right]_+ A_+. \quad (15.a)$$

$$\left[\frac{1}{\rho(z)}\xi\right]_- A_- = \left[\frac{1}{\rho(z)}\xi\right]_+ A_+, \quad \xi = \left(\alpha^{-2}-p^2\right)^{1/2}. \quad (15.b)$$

$$\left[\frac{\cos\theta}{\rho(z)\alpha(z)}\right]_- A_- = \left[\frac{\cos\theta}{\rho(z)\alpha(z)}\right]_+ A_+. \quad (15.c)$$

$$\rho(z_+)\alpha(z_+)\cos\theta_- A_- = \rho(z_-)\alpha(z_-)\cos\theta_+ A_+. \quad (15.d)$$

which differs from equation (14). In fact, with the added condition given above, the reflection coefficient obtained is equivalent to the elastic P̀Ṕ coefficient in Aki and Richards (1980) in the limit $\beta_j \to 0$, β_j being the shear wave velocities. As in the previous case, continuity of pressure requires that $1+R=T$, which is the other condition required to fully specify the coefficient problem at the interface between two acoustic (fluid) media. At this point, it might be useful to conduct finite difference numerical experiments using the radially transformed equations of the acoustic wave equation, the scalar pressure wave equation, and the $S_H -$wave potential equation.

It should be mentioned that the finite difference analogue given in equation (8) may be obtained using the standard method of finite difference analysis (equation B.11) that may be found in many publications on this topic (for example, Mitchell, 1969 or Ames, 1969) and is reviewed briefly in Appendix B for completeness.

NUMERICAL RESULTS

One *FD* program was written with several different internal routines to model the different analogues given above. The results obtained with this software for a simple plane layered model will be compared together with comparisons based on other, less accurate methods such as Asymptotic Ray Theory (ART). The model chosen was such that ART could be used in this study without overly compromising its terms of validity.

However, it maybe useful to return first to plane wave reflection coefficients, specifically the acoustic pressure *PP* reflection coefficient and the scalar potential S_H reflection coefficient at plane interfaces between two media. The acoustic pressure *PP* coefficient obtained from Brekhovskikh (1980) produces the same results if the elastodynamic *PP* reflection coefficient from Aki and Richards (1980) is cautiously used by (numerically) letting the shear wave velocities in both media tend to zero $(\beta_1 = \beta_2 \to 0)$. A more rigorous theoretical pursuit of this indicates that these are equal in the preceding shear wave velocity limit. The *PP* and $S_H S_H$ reflection coefficients (amplitude and phase versus incident angle) are shown in Figures (1) and (2). More discussion is contained in the related figure captions. It is evident that they are quite different especially in the sub-critical region, which is of interest in hydrocarbon seismic prospecting.

For the synthetic trace modeling a single program with two functions was written, where the first function employed equation (6.a) for the acoustic wave, and equation (11) for S_H wave propagation. The disparity in the results for each of these cases may be seen by comparing Figures (3) and (4).

The simple model of a layer over a halfspace chosen to compare the finite difference methods is defined in Table 1. Both the source and receivers are placed at the surface with the plane interface located at a depth of $7.5WL$. The acoustic and S_H wave velocities are both $1WL/T\,(Wavelength/Period)$ and $1.5WL/T$ in the halfspace. A $WL\,(Wavelength)$ and a $T\,(Period)$ are defined relative to a $1500\,m/s$ surface layer velocity and a source pulse predominant frequency of $30Hz$. The densities in the layer and halfspace are $2.0\, gm/cm^3$ and $2.2\, gm/cm^3$, respectively. The receiver offset range is from $(0 \text{ to } 650m; 0 \text{ to } 22.5WL)$ at increments of $10m\,(0.346WL)$. The zero point crossing of the $S_H S_H$ reflection coefficient is located at an offset of approximately $202.5m\,(7WL)$. The critical point in both cases is at an offset of about $390m\,(13.5WL)$. The band limited source wavelet is of the Gabor type. The synthetic traces for these two cases are shown in Figures 3 and 4. As the finite difference scheme is only in the vertical (z) direction and time, 40 points per wavelength were used in the computations.

CONCLUSIONS

Some concepts of finite difference theory for wave propagation in acoustic and elastic (S_H) media were presented. This was done within a hybrid finite difference framework. The finite difference problem consisted of only the depth spatial variable (z) and time. Marginally different finite difference analogues for the second derivative of the potentials $(P \text{ or } S_H)$ with respect to (z) were used with noticeable results which were presented graphically. The extension of what was determined in this simplistic study, to more complicated situations involving hyperbolic systems of partial differential equations, should not be ignored.

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APPENDIX A: FINITE INTEGRAL TRANSFORMS

Although the following finite integral transform methods may be found in the literature (Sneddon, 1972, for example), it was felt that for completeness they should be included here, at least in an abbreviated theorem formulation. The finite Hankel transform of the first kind is a direct application of the following theorem.

Theorem 1: If $f(x)$ satisfies Dirichlet's conditions in the interval $(0,c)$ and if its Hankel transform in that range is defined to be

$$H_\mu\left[f(x)\right] \equiv F(\xi_j) = \int_0^a x\, f(x) J_\mu(\xi_j x)\, dx \qquad \text{(A.1)}$$

where ξ_j is a root of the transcendental equation

$$J_\mu(\xi_j c) = 0 \qquad \text{(A.2)}$$

then, at any point in the interval $(0,a)$ at which the function $f(x)$ is continuous ,

$$f(x) = \frac{2}{c^2} \sum_{j=1}^{\infty} F(\xi_j) \frac{J_\mu(\xi_j x)}{\left[J_{\mu+1}(\xi_j c)\right]^2} \qquad \text{(A.3)}$$

where the sum is taken over all the positive roots of equation (A.2).

APPENDIX B: FINITE DIFFERENCE ANALOGUE

For determining the finite difference analogue in the case of an operation of the type

$$\frac{\partial}{\partial z}\left[\lambda(z)\frac{\partial \phi(z)}{\partial z}\right] \tag{B.1}$$

let

$$w(z)=\lambda(z)\frac{\partial \phi(z)}{\partial z} \tag{B.2}$$

or equivalently

$$w(z)\frac{\partial z}{\lambda(z)}=\partial \phi(z) \tag{B.3}$$

which may be written as

$$w_{n-1/2}\int_{z_{n-1}}^{z_n}\frac{dz}{\lambda(z)}=\phi_n-\phi_{n-1} \tag{B.4}$$

or

$$w_{n-1/2}=\left(\phi_n-\phi_{n-1}\right)\left[\int_{z_{n-1}}^{z_n}\frac{dz}{\lambda(z)}\right]^{-1} \tag{B.5}$$

In a similar manner

$$w_{n+1/2}\int_{z_n}^{z_{n+1}}\frac{dz}{\lambda(z)}=\phi_{n+1}-\phi_n \tag{B.6}$$

or

$$w_{n+1/2}=\left(\phi_{n+1}-\phi_n\right)\left[\int_{z_n}^{z_{n+1}}\frac{dz}{\lambda(z)}\right]^{-1} \tag{B.7}$$

so that

$$\frac{\partial w(z)}{\partial z}=\frac{\partial}{\partial z}\left[\lambda(z)\frac{\partial \phi(z)}{\partial z}\right] \tag{B.8}$$

whose finite difference analogue is of the form

$$\frac{\partial w(z)}{\partial z} \approx \frac{\left(w_{n+1/2} - w_{n-1/2}\right)}{\Delta z} \tag{B.9}$$

which in terms of $\lambda(z)$ and ϕ_n has the form

$$\frac{\partial}{\partial z}\left[\sigma(z)\frac{\partial \phi(z)}{\partial z}\right] \approx \frac{\left(\phi_{n+1} - \phi_n\right)}{\left(\Delta z\right)^2}\left[\frac{1}{\Delta z}\int_{z_n}^{z_{n+1}}\frac{dz}{\sigma(z)}\right]^{-1} - \frac{\left(\phi_n - \phi_{n-1}\right)}{\left(\Delta z\right)^2}\left[\frac{1}{\Delta z}\int_{z_{n-1}}^{z_n}\frac{dz}{\sigma(z)}\right]^{-1}. \tag{B.10}$$

From this it follows that

$$\frac{\partial}{\partial z}\left[\lambda(z)\frac{\partial \phi(z)}{\partial z}\right] \approx \frac{\chi_{n+1}\phi_{n+1} - \left(\chi_{n+1} + \chi_n\right)\phi_n + \chi_n\phi_{n-1}}{\left(\Delta z\right)^2} \tag{B.11}$$

where the χ_k are obtained as

$$\chi_k = \left[\frac{1}{\Delta z}\int_{z_{k-1}}^{z_k}\frac{dz}{\lambda(z)}\right]^{-1} = \frac{2\lambda_k\lambda_{k-1}}{\lambda_k + \lambda_{k-1}} \tag{B.12}$$

using the trapezoidal numerical integration scheme.

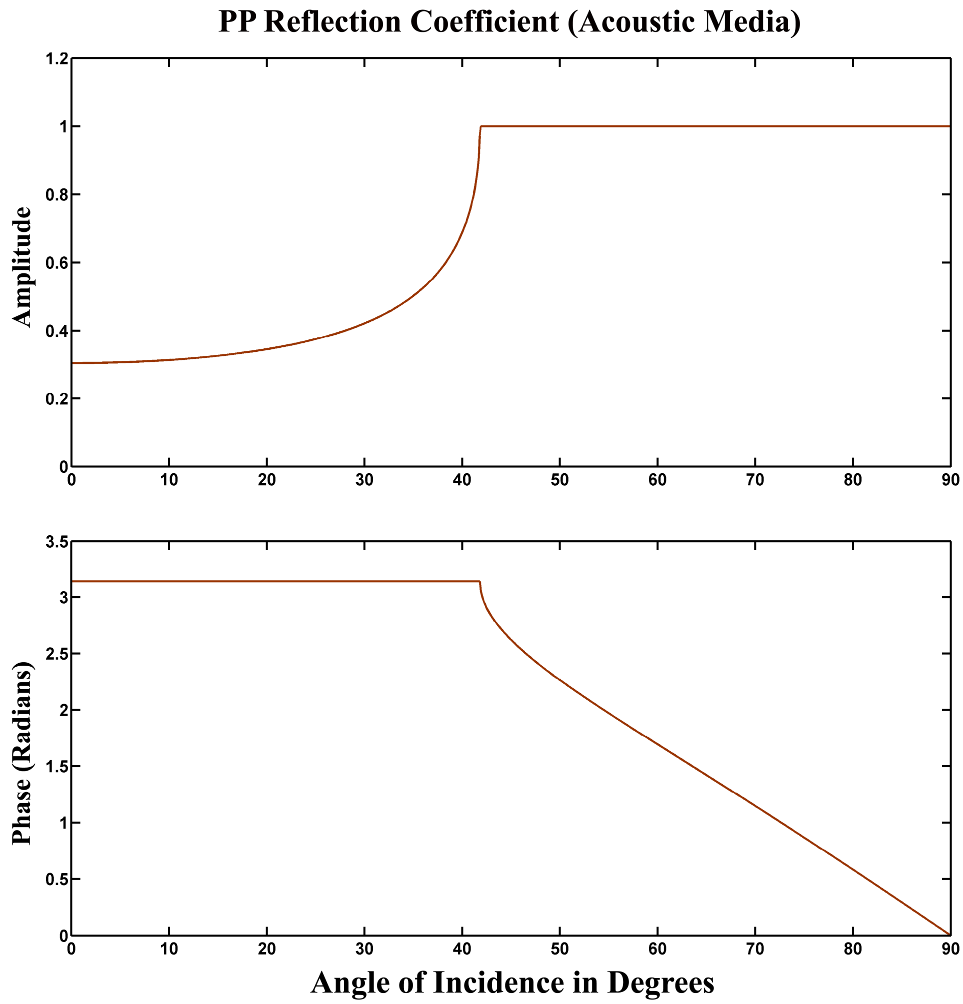

FIG. 1. The acoustic *PP* reflection coefficient at an interface between two acoustic media using elastic constants (velocity and density) given in the text.

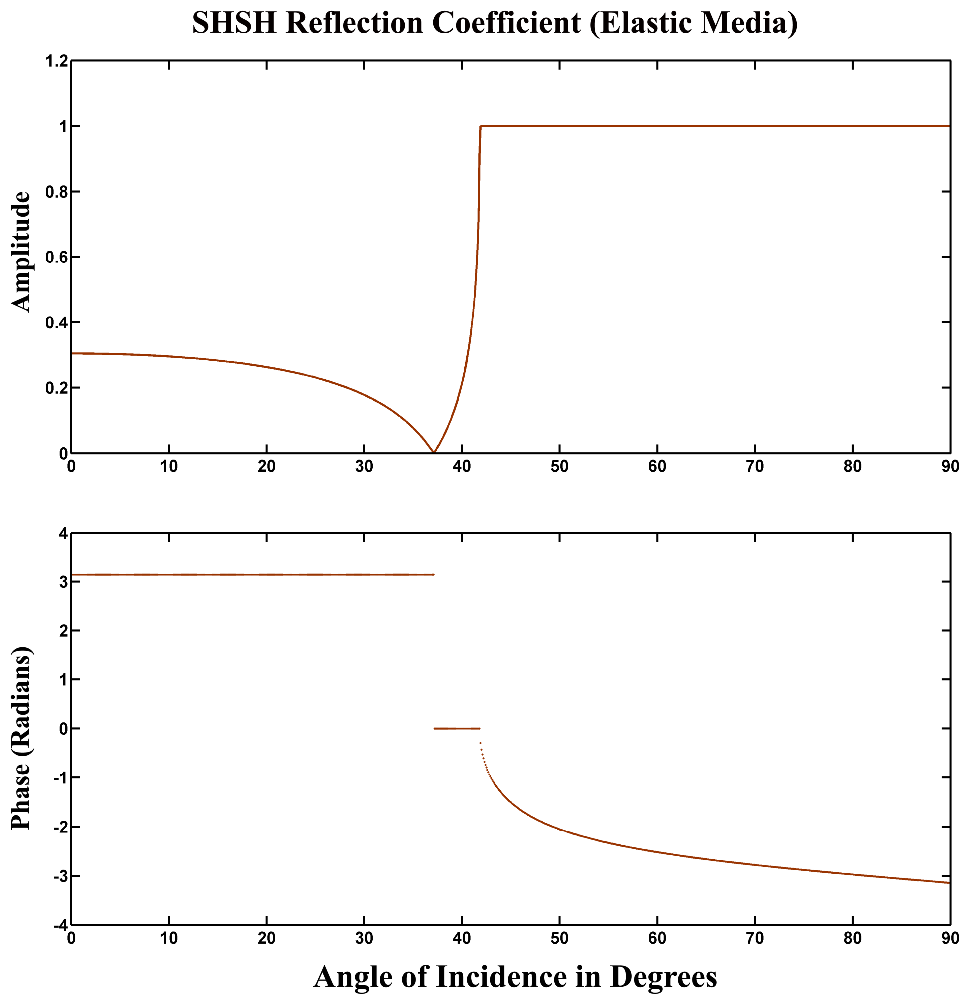

FIG. 2. The $S_H S_H$ reflection coefficient at an interface between two elastic media using constants (velocity and density) given in the text.

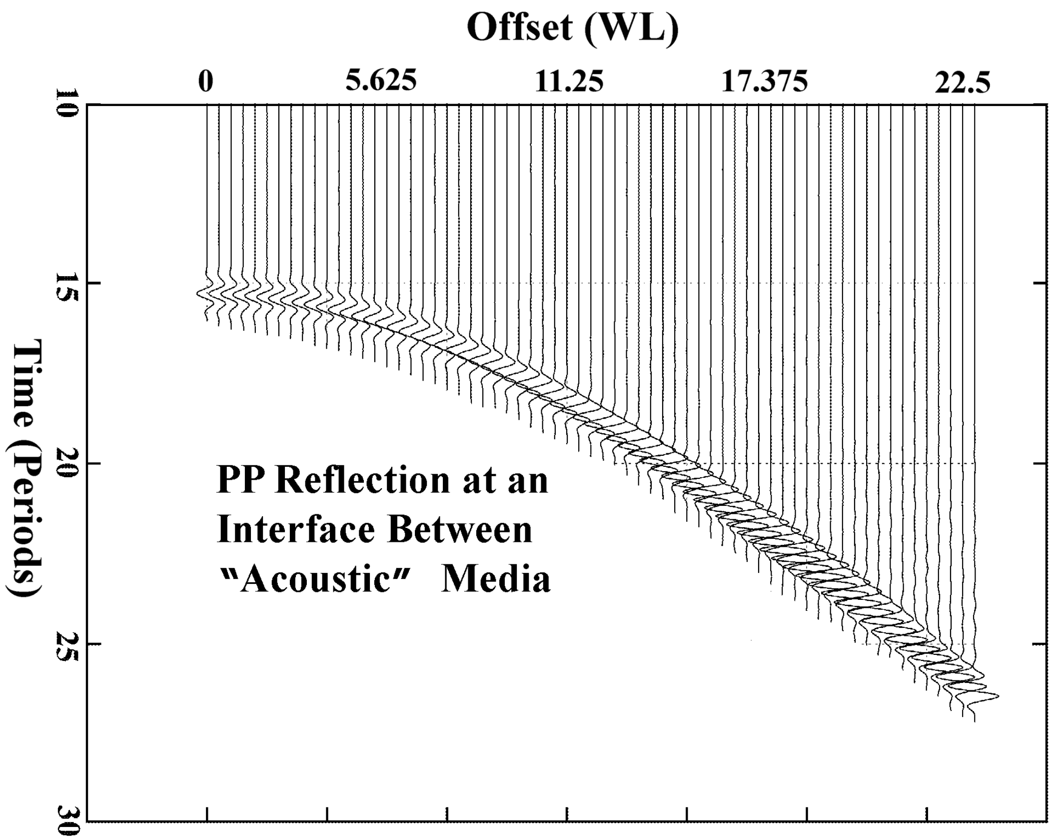

FIG. 3. The reflected *PP* arrival from an interface between two acoustic media. The critically refracted arrival cannot be seen, although some "ringing" at the appropriate offsets is apparent. This appears to be due to the finite difference analogue used.

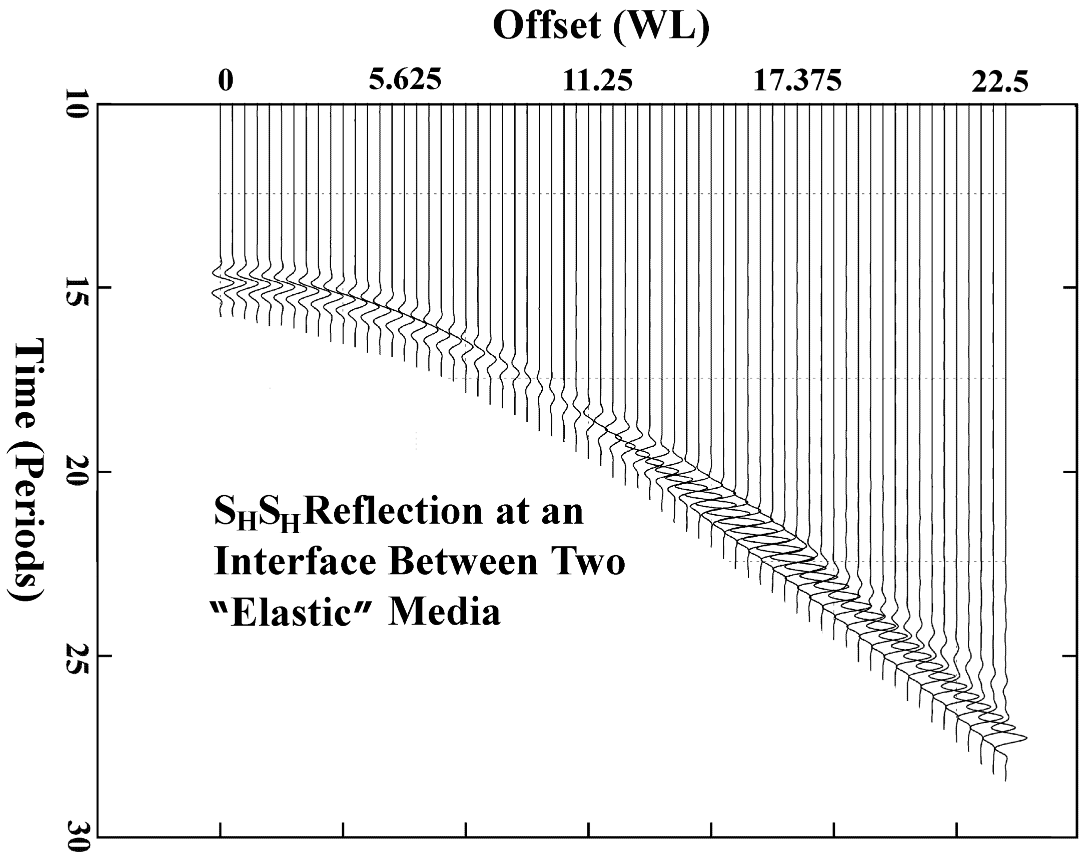

FIG. 4. The reflected S_HS_H (potential) arrival from an interface between two elastic media. The point at which the reflection coefficient passes through zero may be seen, as well as the onset of the critically refracted event at far offset traces.