Coupling ray theory and its quasi–isotropic approximations

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Summary

The contribution is devoted to the numerical calculation of the frequency–dependent complex–valued vectorial amplitudes of S waves in weakly anisotropic media by the coupling ray theory. The efficient and accurate method of numerical integration of the coupling equation is proposed, and the accuracy of the method is estimated in order to control the integration step so, that the relative error in the wavefield amplitudes due to the integration is kept below a given limit. Several quasi–isotropic approximations of the coupling ray theory are briefly discussed and a numerical example is presented.

1 Introduction

There are two different high–frequency asymptotic ray theories, the *isotropic ray theory* assuming equal velocities of both S–wave polarizations and the *anisotropic ray theory* assuming both S–wave polarizations strictly decoupled. In the isotropic ray theory, the S–wave polarization vectors do not rotate around the ray, whereas in the anisotropic ray theory, they coincide with the eigenvectors of the Christoffel matrix which may rotate rapidly around the ray.

In "weakly anisotropic" models, at moderate frequencies, the S–wave polarization tends to stay unrotated round the ray but is partly attracted by the rotation of the eigenvectors of the Christoffel matrix. The intensity of the attraction increases with frequency.

The isotropic and anisotropic ray theories are thus limiting cases and the gap between them has to be filled. A ray theory providing continuous transition between the isotropic and anisotropic ray theories was proposed by Coates & Chapman (1990) and is called the *coupling ray theory*. There are many possible modifications and approximations of the coupling ray theory. For example, the reference ray may be calculated in different ways (Bakker 2001), the Christoffel matrix may be approximated by its quasi–isotropic projections onto the plane perpendicular to the reference ray and onto the tangent line to the reference ray (Pšenčík 1998; Červený 1998, 2001), travel times corresponding to the anisotropic ray theory may be approximated in several ways, e.g. by linear quasi–isotropic perturbation with respect to the density–normalized elastic parameters (Pšenčík 1998; Červený 1998, 2001), etc. Several quasi–isotropic approximations of the coupling ray theory are briefly discussed in Section 6.

For comparison of isotropic, anisotropic and coupling ray theories with the exact solution in a simple model refer to Bulant, Klimeš & Pšenčík (2000). The comparison also includes the quasi–isotropic approximation of the coupling ray theory by Pšenčík (1998), especially the effect of quasi–isotropic approximation of travel times by linear perturbation with respect to the elastic parameters. The effect of the quasi–isotropic approximation of the Christoffel matrix is demonstrated on the numerical example in this expanded abstract, see Section 7. Both the computer code and data for the calculation are available.

The numerical algorithm of calculation of the frequency–dependent complex–valued S–wave polarization vectors of the coupling ray theory is proposed. The method of numerical integration of the coupling equation, proposed by Červený (1998, 2001), is applied to the coupling equation derived by Coates & Chapman (1990), with emphasis on the numerical implementation. The method of integration does not need to calculate angular velocity $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ of the rotation of the eigenvectors of the Christoffel matrix along the reference ray and does not require $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ to be smooth or finite along the reference ray. This is important property, because the angular velocity of the rotation is undefined in singular regions of two equal eigenvalues of the Christoffel matrix.

The accuracy of the method of numerical integration of the coupling equation described in Section 5 enables to control the integration step so, that the relative error in the wavefield amplitudes due to the integration is kept below a given limit, which is of principal importance for numerical applications.

2 Coupling ray theory for S waves

Assume a curve in phase space, hereinafter called the "reference ray", parametrized by reference travel time τ, with reference slowness vectors $p_i(\tau)$ known at all its points $x_j(\tau)$. The reference ray should be close to the ray of the wave under study. In particular, if shear wave coupling in weakly anisotropic media is investigated and the same reference ray is used for both S–wave polarizations, the reference ray should be close to the high–frequency approximations of the rays of both S waves (Bakker 2001).

Using the reference slowness vectors, we can calculate Christoffel matrices

$$\Gamma_{jk}(\tau) = p_i(\tau)\, a_{ijkl}\,(x_j(\tau))\; p_l(\tau) \tag{1}$$

and their eigenvectors $g_{i1}(\tau)$, $g_{i2}(\tau)$, $g_{i3}(\tau)$ along the reference ray. Assume that eigenvectors $g_{i1}(\tau)$ and $g_{i2}(\tau)$ correspond to S waves and that they vary continuously along the reference ray. The continuity is not required in the regions where the corresponding two eigenvalues are equal. Let us denote $\tau_1(\tau)$ and $\tau_2(\tau)$ the travel times corresponding to polarizations $g_{i1}(\tau)$ and $g_{i2}(\tau)$, respectively. They may be approximated by quadratures along the unperturbed reference ray,

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau} = [\Gamma_{jk} g_{j1} g_{k1}]^{-\frac{1}{2}} \ , \quad \frac{\mathrm{d}\tau_2}{\mathrm{d}\tau} = [\Gamma_{jk} g_{j2} g_{k2}]^{-\frac{1}{2}} \ . \tag{2}$$

The coupling ray theory solution u_i of the elastodynamic equations may then be expressed, for S waves, as a linear combination of the anisotropic ray theory solutions (Coates & Chapman 1990, eq. 15),

$$u_i = \sum_{M=1}^{2} g_{iM}\, A_M\, r_M \exp(\mathrm{i}\omega\tau_M) \quad , \tag{3}$$

where $A_M = A_M(\tau)$ are the complex–valued scalar amplitudes in the high–frequency approximation corresponding to polarizations g_{iM}. Because the amplitudes are calculated for the selected system of reference rays, using the relevant dynamic ray tracing along the reference ray (Červený 1972), they are identical, $A_M \equiv A = A(\tau)$. The coupling ray theory equation for complex–valued factors $r_M = r_M(\tau)$ reads (Coates & Chapman 1990, eq. 30)

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = \frac{\mathrm{d}\varphi}{\mathrm{d}\tau}\begin{pmatrix} 0 & E \\ -E^* & 0 \end{pmatrix}\begin{pmatrix} r_1 \\ r_2 \end{pmatrix} \quad , \tag{4}$$

where

$$\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} = g_{k2}\frac{\mathrm{d}g_{k1}}{\mathrm{d}\tau} = -g_{k1}\frac{\mathrm{d}g_{k2}}{\mathrm{d}\tau} \tag{5}$$

is the angular velocity of the eigenvector rotation, and

$$E = \exp\left(\mathrm{i}\omega[\tau_2(\tau) - \tau_1(\tau)]\right) \quad . \tag{6}$$

For several possible modifications and approximations of the above formulation of the coupling ray theory refer to Section 6.

For high frequencies, $\exp\left(\mathrm{i}\omega[\tau_2(\tau) - \tau_1(\tau)]\right)$ in equation (4) may oscillate rapidly. These oscillations have no high–frequency impact on the solution because they cancel out after each period and the derivative of the solution is zero on average at high frequencies. However, these oscillations may either considerably reduce the accuracy, or increase the cost of the numerical integration. In addition, travel times τ_M in equation (4) depend on the initial conditions. Equation (4) is thus much less suitable for defining the propagator matrix than equations with purely local coefficients.

The oscillation and global character of the coefficient matrix of equation (4) is caused by different travel times τ_M with respect to which the amplitude factors r_M are defined. Let us introduce new amplitude factors a_M, both related to the same "average" travel time $\overline{\tau}$ (Červený 1998, 2001),

$$r_1\exp(\mathrm{i}\omega\tau_1) = a_1\exp(\mathrm{i}\omega\overline{\tau})\ ,\ \ r_2\exp(\mathrm{i}\omega\tau_2) = a_2\exp(\mathrm{i}\omega\overline{\tau})\ . \tag{7}$$

Inserting $r_M = a_M \exp\left(\mathrm{i}\omega[\overline{\tau} - \tau_M]\right)$ into equation (4), we obtain equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \mathbf{B}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad , \tag{8}$$

where

$$\mathbf{B} = \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} - \mathrm{i}\omega\begin{pmatrix} \frac{\mathrm{d}(\overline{\tau}-\tau_1)}{\mathrm{d}\tau} & 0 \\ 0 & \frac{\mathrm{d}(\overline{\tau}-\tau_2)}{\mathrm{d}\tau} \end{pmatrix}\right] \quad . \tag{9}$$

It seems reasonable to simplify equation (8) by choosing

$$\overline{\tau}(\tau) = \tfrac{1}{2}[\tau_1(\tau) + \tau_2(\tau)] \quad . \tag{10}$$

Coefficient matrix (9) of equation (8) then takes the form

$$\mathbf{B} = \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} - \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}\frac{\omega}{2}\frac{\mathrm{d}(\tau_2 - \tau_1)}{\mathrm{d}\tau}\right] \quad . \tag{11}$$

3 Propagator matrix

Propagator matrix Π^g of equation (11), defined as

$$\Pi^g_{MN}(\tau,\tau_0) = \frac{\partial\, a_M(\tau)}{\partial\, a_N(\tau_0)} \quad , \tag{12}$$

is a complex–valued 2×2 matrix satisfying equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\Pi^g = \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{\mathrm{d}\varphi}{\mathrm{d}\tau} - \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}\frac{\mathrm{d}\epsilon}{\mathrm{d}\tau}\right]\Pi^g \ , \tag{13}$$

directly following from equation (11). Here

$$\epsilon(\tau) = \tfrac{1}{2}\omega\ [\tau_2(\tau) - \tau_1(\tau)] \quad . \tag{14}$$

Propagator matrix Π^g is symplectic and unitary, but we do not need to make use of these properties in this contribution.

It is difficult to integrate equation (13) by Runge–Kutta or another numerical method which requires to calculate derivative $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ along the reference ray, because this derivative is undefined in singular regions of two equal eigenvalues of Christoffel matrix (1). The method of integration proposed in this expanded abstract does not need to calculate derivative $\frac{\mathrm{d}\varphi}{\mathrm{d}\tau}$ and does not require the derivative to be smooth or finite along the reference ray.

Since Π^g is a propagator matrix satisfying the chain rule, it may be numerically calculated as the product of propagator matrices Π^g corresponding to reasonably small segments of the reference ray (Červený 1998, 2001). Frequency–dependent propagator matrices along individual small ray segments may be approximated with various degrees of accuracy and efficiency.

4 Approximation for short ray segments

The approximate local solution of coupling equation (13) with unit initial conditions has been derived by Bulant & Klimeš (1998) and Červený (1998, 2001) in the form of

$$\boxed{\Pi^g(\tau,\tau_0) = \exp\left(\mathbf{A}\Delta\alpha\right) = \mathbf{1}\cos(\Delta\alpha) + \mathbf{A}\sin(\Delta\alpha)\ ,} \tag{15}$$

where

$$\boxed{\mathbf{A} = \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\Delta\varphi - \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}\Delta\epsilon\right](\Delta\alpha)^{-1}} \tag{16}$$

and

$$\boxed{\Delta\alpha = \sqrt{(\Delta\varphi)^2 + (\Delta\epsilon)^2} \quad .} \tag{17}$$

Here we have put

$$\Delta\varphi = \varphi(\tau) - \varphi(\tau_0)\ , \quad \Delta\epsilon = \epsilon(\tau) - \epsilon(\tau_0)\ . \tag{18}$$

We now suggest how to calculate $\Delta\varphi$ and $\Delta\epsilon$ and how to control the accuracy of the approximation.

The approximation of $\Delta\varphi$, based on equation (5), is (Bulant & Klimeš 1998)

$$\Delta\varphi = \arctan\left(\frac{g_{k1}(\tau)g_{k2}(\tau_0) - g_{k2}(\tau)g_{k1}(\tau_0)}{g_{k1}(\tau)g_{k1}(\tau_0) + g_{k2}(\tau)g_{k2}(\tau_0)}\right) \quad . \tag{19}$$

Travel times τ_M, $M = 1, 2$, can be obtained by trapezoidal quadratures of equations (2),

$$\Delta\tau_M = \tau_M(\tau) - \tau_M(\tau_0) \approx \tfrac{1}{2}\left[\tfrac{\mathrm{d}\tau_M}{\mathrm{d}\tau}(\tau) + \tfrac{\mathrm{d}\tau_M}{\mathrm{d}\tau}(\tau_0)\right]\Delta\tau\ . \tag{20}$$

Equations (10) and (14) then yield

$$\Delta\overline{\tau} = \tfrac{1}{2}(\Delta\tau_2 + \Delta\tau_1)\ , \quad \Delta\epsilon = \tfrac{1}{2}\,\omega\,(\Delta\tau_2 - \Delta\tau_1)\ . \tag{21}$$

The propagator matrix of coupling equation (13) is numerically calculated as the product of matrices (15) corresponding to individual steps of numerical integration. The accuracy of approximate local solution (15) have been estimated by Bulant & Klimeš (1998) in order to control the integration step so, that the relative error in the wavefield amplitudes due to the integration is kept below a given limit.

5 Accuracy of the approximation

To keep the error in Π^g along the whole ray of length τ (measured in travel time) below the maximum specified limit δ, we require

$$\boxed{|\Delta\varphi|\left|\Delta\frac{\mathrm{d}\tau_2}{\mathrm{d}\tau} - \Delta\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau}\right| \le \frac{12}{\omega\tau}\,\delta \quad ,} \tag{22}$$

see (2). Note that, in addition to inequality (22), step $\Delta\varphi$ in the eigenvector rotation must also be sufficiently smaller than 45°,

$$|\Delta\varphi| \ll \frac{\pi}{4} \quad , \tag{23}$$

in order to reliably follow the selected eigenvector g_{kM} along the reference ray. Condition (23) need not be satisfied in the regions where the corresponding two eigenvalues are equal, i.e. where $\Delta\epsilon = 0$ within required numerical accuracy. For example, there is no restriction on the selection of the eigenvectors of the Christoffel matrix in the isotropic parts of the model, while the proposed integration of the coupling equation is accurate. Inequality (22) can be satisfied in smooth models without problems, independently of the degree of anisotropy.

6 Quasi–isotropic approximations of the coupling ray theory

6.1 Selection of the reference ray

The isotropic ray theory is always the limiting case of the coupling ray theory for decreasing anisotropy at fixed frequency. On the other hand, the high–frequency limit of the coupling ray theory at fixed anisotropy is dependent on the choice of the reference ray, and even on the choice of the *system* of reference rays, because the amplitudes are determined by the paraxial reference rays.

If we choose the *anisotropic ray theory reference ray* and select the initial polarization corresponding to the reference ray, the coupling ray theory will correctly limit to the anisotropic ray theory for high–frequencies. For other choices of reference rays, the high–frequency limit of the coupling ray theory at fixed anisotropy is incorrect, although the differences may be negligible at finite frequencies under consideration.

In the *anisotropic common–ray approximation*, the common reference ray is traced using the averaged Hamiltonian of both S–wave polarizations (Bakker 2001).

In less accurate *isotropic common–ray approximation*, the reference ray is traced in the reference isotropic model. Moreover, the reference isotropic model may be selected in different ways, yielding quasi–isotropic approximations of various accuracy.

6.2 Quasi–isotropic projection of the polarization vectors

The coupling ray theory solution (3) may be approximated by its projection

$$\tilde{u}_i = h_{iM} h_{mM} u_m \tag{24}$$

onto the orthonormal reference polarization vectors h_{k1}, h_{k2}. This approximation may simplify modification of existing isotropic ray tracing codes for the coupling ray theory. The error of this approximation is obvious and can simply be calculated.

6.3 Quasi–isotropic approximation of the Christoffel matrix

Denote here h_{k1}, h_{k2} and h_{k3} the polarization vectors of the isotropic ray theory, or the reference polarization vectors in general. If the Christoffel matrix is approximated by its projections onto plane span$\{h_{i1}, h_{j2}\}$ and onto vector h_{k3},

$$\begin{aligned}\tilde{\Gamma}_{jk} &= h_{jM} h_{mM} \Gamma_{mn} h_{nN} h_{kN} + h_{j3} h_{m3} \Gamma_{mn} h_{n3} h_{k3} \\ &= \Gamma_{jk} - (h_{jM} h_{k3} + h_{j3} h_{kM}) h_{mM} \Gamma_{mn} h_{n3} \quad ,\end{aligned} \tag{25}$$

eigenvectors g_{i1} and g_{j2} get situated in plane span$\{h_{i1}, h_{j2}\}$ as in the quasi–isotropic approximation of Pšenčík (1998) and Červený (1998, 2001). This approximation includes the approximation of Section 6.2.

6.4 Quasi–isotropic perturbation of travel times

Linearized perturbation of equations (2) with respect to the density–normalized elastic parameters yields approximation

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau} \approx (\Gamma^0_{jk} g_{j1} g_{k1})^{-\frac{1}{2}} - \frac{1}{2}(\Gamma_{jk} - \Gamma^0_{jk}) g_{j1} g_{k1} (\Gamma^0_{jk} g_{j1} g_{k1})^{-\frac{3}{2}} . \tag{26}$$

Assuming that $\Gamma^0_{jk} g_{j1} g_{k1} = 1$, see Section 6.3, equation (26) reads

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau} \approx \frac{3}{2} - \frac{1}{2}\Gamma_{jk} g_{j1} g_{k1} \quad , \tag{27}$$

as in the quasi–isotropic approximation of Pšenčík (1998) and Červený (1998, 2001). Analogously for $\frac{\mathrm{d}\tau_2}{\mathrm{d}\tau}$.

7 Numerical example

A 1-D anisotropic model QI (model WA rotated by 45°) was provided by Pšenčík & Dellinger (2001) who performed the coupling ray theory calculations using the programs of package ANRAY. The normalized elastic parameters a_{ijkl} and reference velocities are specified at the surface (zero depth) and at the depth of 1 length unit, and are interpolated linearly with depth. The reference isotropic model is given by $v_\mathrm{P}^2 = 15.00$ & $v_\mathrm{S}^2 = 5.10$ at the surface, and $v_\mathrm{P}^2 = 23.00$ & $v_\mathrm{S}^2 = 7.79$ at the depth of 1 length unit. The homogeneous density is $\rho = 1$. The synthetic seismograms, corresponding to vertical force $\mathbf{F} = (0, 0, 100)^\mathrm{T}$ at position $(50, 50, 0)^\mathrm{T}$, are calculated at 29 receivers $(51, 50, 0.010)^\mathrm{T}$, $(51, 50, 0.030)^\mathrm{T}$, $(51, 50, 0.050)^\mathrm{T}$, ..., $(51, 50, 0.570)^\mathrm{T}$ located in a vertical well. The source time function is the Gabor signal $\cos(2\pi f t)\exp[-(2\pi f t/4)^2]$ with reference frequency $f = 50\,\mathrm{Hz}$, band–pass filtered by cosine filter given by frequencies 0 Hz, 5 Hz, 60 Hz and 100 Hz.

The resulting coupling ray theory seismograms (calculated by package CRT), modified by the quasi–isotropic projection of Section 6.2 are plotted in Figure 1 by a solid line. The maximum polarization error of the quasi–isotropic projection is 0.061 radians in this example. For comparison, the seismograms calculated according to the quasi–isotropic approximation of Section 6.3 (corresponding to the seismograms calculated by package ANRAY) are plotted by a dotted line. The effect of the quasi–isotropic approximation of Section 6.4 is negligible in this example. On the other hand, the effect of the quasi–isotropic approximation of Section 6.4 has been demonstrated by Bulant, Klimeš & Pšenčík (2000) in a simple model in which the quasi–isotropic approximation of Section 6.3 does not affect the results.

The model is named QI and the data for packages CRT and ANRAY may be found on compact disks Klimeš (1998), Bucha & Klimeš (1999) and Bucha, Bulant & Klimeš (2000), together with the Fortran 77 source code of the packages. For comparison with the isotropic and anisotropic ray theory seismograms and for more detailed discussion and description of this model refer to Pšenčík & Dellinger (2001).

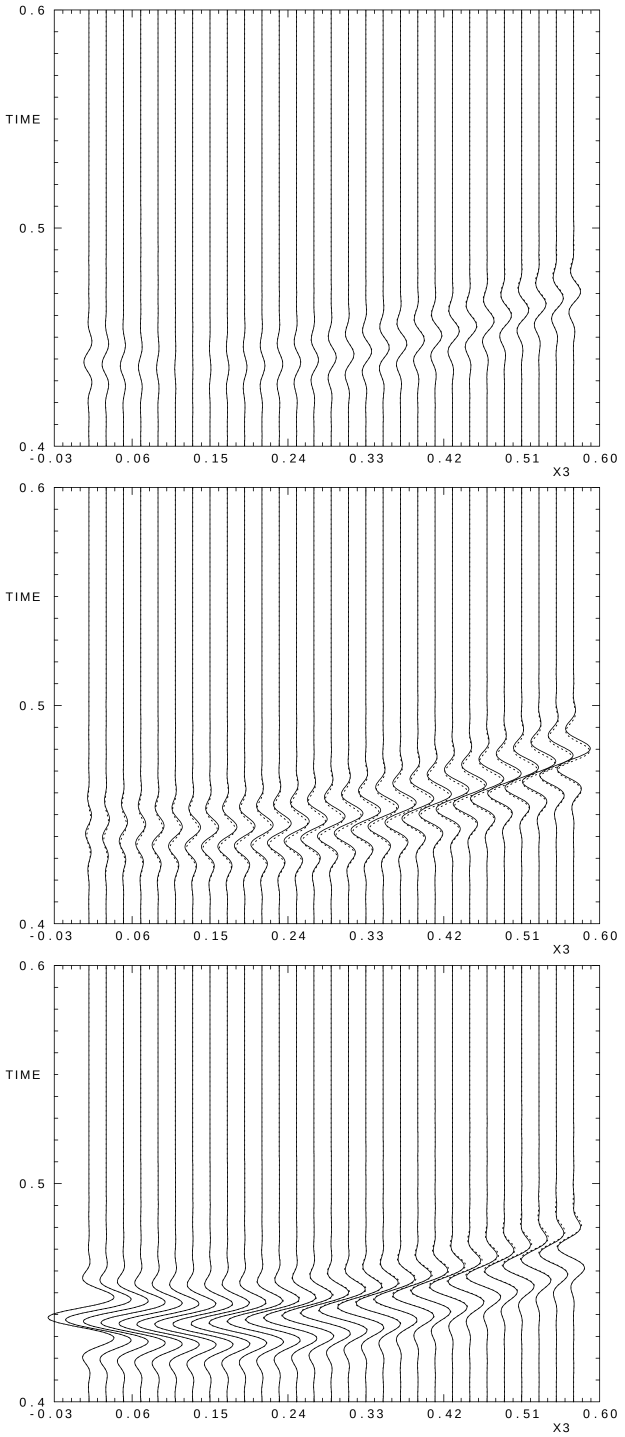

Figure 1. From the top to the bottom: the first (radial), second (transverse) and third (vertical) component of the synthetic seismograms. The coupling ray theory seismograms are plotted by the solid line. The dotted seismograms correspond to the quasi–isotropic approximation of the Christoffel matrix. Note that the second (transverse) component is zero in the one–dimensional reference isotropic model.

8 Conclusions

The proposed numerical algorithm for the coupling ray theory is very efficient and accurate, with controlled accuracy. It requires negligible computational time because the coupling equation is solved only along the previously calculated two–point rays. In weakly anisotropic media, the coupling ray theory should be much more accurate than the isotropic and anisotropic ray theories, although its actual accuracy and limits of applicability are still unknown.

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* Available online at "http://seis.karlov.mff.cuni.cz/consort/main.htm".