Errors due to the common ray approximations of the coupling ray theory

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Summary

The equations for estimating the travel–time errors due to the isotropic and anisotropic common ray approximations of the coupling ray theory for S waves are presented and numerically tested.

1. Introduction

The *coupling ray theory*, applicable at all degrees of anisotropy, from isotropic models to considerably anisotropic ones, has been proposed by Coates & Chapman (1990). The numerical algorithm for calculating the frequency–dependent complex–valued S–wave polarization vectors of the coupling ray theory has been designed by Bulant & Klimeš (2002a).

There are many commonly used *quasi–isotropic approximations* of the coupling ray theory (Pšenčík 1998a), which deteriorate the accuracy of the coupling ray theory both with increasing frequency and increasing degree of anisotropy. Most of these quasi–isotropic approximations can be avoided with minimal effort (Bulant & Klimeš 2002a), except for the *common ray approximation* for S waves. In the common ray approximation, only one reference ray is traced for both S–wave polarizations, and both S–wave travel times are approximated by the perturbation from the common reference ray. The common ray approximation thus considerably simplifies the coding of the coupling ray theory and numerical calculations, but may introduce errors in travel times due to the perturbation. These travel–time errors can deteriorate the coupling ray theory solution at high frequencies. It is thus of principal importance for numerical applications to estimate the error due to the common ray approximation.

In the common ray approximation, the S–wave travel times are usually approximated by the linear perturbation from the common reference ray. The errors of S–wave travel times may then be approximated by second–order perturbations. The calculation of these estimates of travel–time errors due to the *isotropic common ray approximation* and the *anisotropic common ray approximation* (Bakker 2002) is proposed and numerically demonstrated in this paper. The estimates are based on the equations for the second–order perturbations of travel time derived by Klimeš (2002). For the derivation of the coupling ray theory refer to Coates & Chapman (1990) and Červený (2001). For the description of the numerical algorithm refer to Bulant & Klimeš (2002a). For more detailed description of the common ray approximations of the coupling ray theory refer to Klimeš & Bulant (2002). For other quasi–isotropic approximations of the coupling ray theory refer to Bulant & Klimeš (2002b).

2. Common ray approximations

The reference ray should be close to the ray of the wave under study. In particular, the reference ray is best represented by the *anisotropic ray theory reference ray*, with the initial condition for the vectorial amplitude given by the relevant eigenvector of the Christoffel matrix corresponding to the reference ray. Then the travel time of the selected polarization is exact, and only the travel–time difference between the S–wave polarizations is approximate. The coupling ray theory may then also be used at high frequencies because the approximate travel–time difference influences only the coupling due to low–frequency scattering. The coupling ray theory then correctly limits to the anisotropic ray theory for high frequencies. For other choices of reference rays, the high–frequency limit of the coupling ray theory at a fixed anisotropy is incorrect.

In the *anisotropic common ray approximation*, the common reference ray is traced using the averaged Hamiltonian of both S–wave polarizations (Bakker 2002).

In the 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.

3. Linear perturbation of travel time

Let $a_{ijkl} = a_{ijkl}(x_m)$ be the density–normalized elastic moduli describing a *smooth anisotropic model*, and $v_0 = v_0(x_m)$ the velocity in the smooth *reference isotropic model* used to trace the reference rays. We shall abbreviate v_0 as the reference velocity. Assume a phase–space *reference ray*, parametrized by reference travel time τ, with reference slowness vectors $p_i(\tau)$ known at all its points $x_j(\tau)$. Using the reference slowness vectors, we can calculate reference Christoffel matrix

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

and its eigenvectors $g_{i\alpha}(\tau)$, $\alpha = 1, 2, 3$ along the reference ray. Whereas the Einstein summation over the pairs of identical Roman indices (both subscripts and superscripts) $i, j, k, ... = 1, 2, 3$ or $I, J, K, ... = 1, 2$ is used throughout this paper, no implicit summation applies to Greek subscripts $\alpha, \beta, ...$ indexing the eigenvectors of the Christoffel matrix. Assume that eigenvectors $g_{i1}(\tau)$ and $g_{i2}(\tau)$ correspond to the S waves, and eigenvector $g_{i3}(\tau)$ to the P wave. The eigenvectors should vary continuously along the reference ray. Let us denote $\tau_\alpha(\tau)$ the travel time corresponding to the selected polarization $g_{i\alpha}(\tau)$. It may be approximated by a quadrature along the unperturbed reference ray,

$$\frac{\mathrm{d}\tau_\alpha}{\mathrm{d}\tau} = [\Gamma_{jk} g_{j\alpha} g_{k\alpha}]^{-\frac{1}{2}} \quad . \tag{2}$$

Travel–time approximation (2), suggested for the coupling ray theory by Bulant & Klimeš (2002a), would become exact for a reference ray following the path of the exact ray.

4. Correct and reference Hamiltonians

Travel–time approximation (2) can be derived as the linear perturbation corresponding to Hamiltonian

$$H_\alpha(x_m, p_n) = -[G_\alpha(x_m, p_n)]^{-\frac{1}{2}} \quad , \tag{3}$$

where $G_\alpha(x_m, p_n)$ is the eigenvalue of Christoffel matrix (1), corresponding to polarization $g_{i\alpha}$ (Klimeš 2002, eqs. 43 and 65). The value of Hamiltonian (3), corresponding to unit eigenvector $g_{i\alpha}$ of the Christoffel matrix, at the reference ray, is

$$H_\alpha = -(a_{ijkl} g_{i\alpha} p_j g_{k\alpha} p_l)^{-\frac{1}{2}} \quad . \tag{4}$$

Hamiltonian (3), specified for the reference isotropic medium, reads

$$H_0(x_m, p_n) = -[v_0(x_m)]^{-1} (p_i p_i)^{-\frac{1}{2}} \quad . \tag{5}$$

We shall now specify the partial derivatives of the Hamiltonians (3) and (5) at the reference ray, required for esimating the accuracy of the common ray approximations,

$$H_{0,i} = v_{0,i} (v_0)^{-1} \quad , \tag{6}$$

$$H_{\alpha,i} = -\tfrac{1}{2} (H_\alpha)^3 a_{mjkl,i} g_{m\alpha} p_j g_{k\alpha} p_l \quad . \tag{7}$$

$$H_\alpha^{,i} = -(H_\alpha)^3 a_{mikl} g_{m\alpha} g_{k\alpha} p_l \quad . \tag{8}$$

The derivatives with respect to the coordinates are denoted by Roman subscripts following a comma, Partial derivatives with respect to the components of the slowness vector are denoted by Roman superscripts following a comma.

5. Parametric system of the Hamiltonians and errors due to the common ray approximations

We consider the two–parametric set $H = H(x_m, p_n, f_\alpha)$ of Hamiltonians parametrized by f_α, $\alpha = 1, 2$ for an S wave, or the one–parametric set $H = H(x_m, p_n, f_\alpha)$ of Hamiltonians parametrized by f_α, $\alpha = 3$ for a P wave,

$$\begin{aligned} H(x_m, p_n, f_\alpha) &= H_0(x_m, p_n) \\ &\quad + \sum_\alpha [H_\alpha(x_m, p_n) - H_0(x_m, p_n)]\, f_\alpha \;. \end{aligned} \tag{9}$$

Parametric system (9) of the Hamiltonians then generates parametric system $\tau(x_m, f_\alpha)$ of travel time fields corresponding to the individual Hamiltonians $H(x_m, p_n, f_\alpha)$.

For an S wave, we obtain the Hamiltonian corresponding to the isotropic common ray approximation in the reference isotropic model for $(f_1, f_2) = (0, 0)$, the Hamiltonian corresponding to the first anisotropic S–wave polarization for $(f_1, f_2) = (1, 0)$, the Hamiltonian corresponding to the second anisotropic S–wave polarization for $(f_1, f_2) = (0, 1)$, and the averaged Hamiltonian of both S–wave polarizations corresponding to the anisotropic common ray approximation by Bakker (2002) for $(f_1, f_2) = (\frac{1}{2}, \frac{1}{2})$.

For a P wave, we obtain the Hamiltonian corresponding to the reference ray in the reference isotropic model for $f_3 = 0$, and the Hamiltonian corresponding to the anisotropic P wave for $f_3 = 1$.

The second–order Taylor expansion of travel time with respect to parameters f_α is

$$\tau(\bullet, f_\alpha) \approx \tau + \sum_\alpha \tau_{,\alpha} f_\alpha + \tfrac{1}{2} \sum_\alpha \sum_\beta \tau_{,\alpha\beta} f_\alpha f_\beta \quad , \tag{10}$$

where the Greek subscripts following a comma denote the derivatives with respect to parameters f_α, also called *perturbations*. Here travel time τ and its perturbations $\tau_{,\alpha}$, $\tau_{,\alpha\beta}$ written without arguments f_α correspond to the reference model $f_\alpha = 0$. Travel–time approximation (2) corresponds to the linear part of Taylor expansion (10). The error of travel–time approximation (2) may thus be approximated by the second–order term in Taylor expansion (10).

We may now express the estimates of the travel–time errors due to the *isotropic common ray* (ICR) *approximation* of anisotropic travel times in terms of the second–order perturbations of travel time. The errors of travel–time approximation (2) from isotropic common reference ray $(f_1, f_2) = (0, 0)$ to the correct anisotropic S–wave ray $(f_1, f_2) = (1, 0)$ and to the correct anisotropic S–wave ray $(f_1, f_2) = (0, 1)$ are approximately

$$\delta\tau_\alpha^{\rm ICR} = \frac{\tau_{,\alpha\alpha}}{2} \quad , \tag{11}$$

where $\alpha = 1, 2$ for S waves. Equation (11) with $\alpha = 3$ gives analogously the estimate of the error of travel–time approximation (2) from isotropic reference P–wave ray $f_3 = 0$ to the correct anisotropic P–wave ray $f_3 = 1$.

We may also use the second–order perturbations of travel time, calculated along the isotropic common reference ray, to estimate the accuracy of the *anisotropic common ray* (ACR) *approximation* (Bakker 2002). The estimates of errors of travel–time approximation (2) from anisotropic S–wave common reference ray $(f_1, f_2) = (\frac{1}{2}, \frac{1}{2})$ to $(f_1, f_2) = (1, 0)$ and to $(f_1, f_2) = (0, 1)$ are equal,

$$\delta\tau_\alpha^{\rm ACR} = \frac{\tau_{,11} - 2\tau_{,12} + \tau_{,22}}{8} \quad , \tag{12}$$

where $\alpha = 1, 2$. Error estimates (12) represent the contributions of the quadratic terms in Taylor expansion (10) at the distances from the anisotropic S–wave common reference ray to the correct S–wave rays.

6. Ray-centred coordinates, dynamic ray tracing

Let us denote by h_{i1}, h_{i2}, h_{i3} the basis vectors of the *ray–centred coordinate system* (Riemannian normal coordinate system). The orthonormal basis vectors of the ray–centred coordinate system are calculated along the reference ray in the reference isotropic model. The first two basis vectors h_{iM} of the ray–centred coordinate system are tangent to the wavefront, the third basis vector $h_{i3} = v_0 p_i$ is tangent to the ray. The equations for calculating the basis vectors of the ray–centred coordinate system can be found, e.g., in the book by Červený (2001).

The quantities covariantly transformed from spatial coordinates x_i to the local Cartesian basis h_{im} of the ray–centred coordinate system are marked by a tilde $\tilde{}$. In particular,

$$\widetilde{H}_{0,i} = H_{0,m} h_{mi} \ , \ \ \widetilde{H}_{\alpha,i} = H_{\alpha,m} h_{mi} \ , \ \ \widetilde{H}_\alpha^{,i} = H_\alpha^{,m} h_{mi} \ . \tag{13}$$

The 2×2 transformation matrices $\widetilde{Q}_{IJ}$ and $\widetilde{P}_{IJ}$, from ray take–off parameters γ_J to ray–centred coordinates q_I and to the slowness–vector components $\widetilde{p}_i$ in the ray–centred coordinate system, can be calculated by the *dynamic ray tracing equations in ray–centred coordinates* (Červený 2001, eq. 4.1.65),

$$\frac{\rm d}{{\rm d}\tau} \widetilde{Q}_{IJ} = (v_0)^2 \ \widetilde{P}_{IJ} \quad . \tag{14}$$

$$\frac{\rm d}{{\rm d}\tau} \widetilde{P}_{IJ} = -(v_0)^{-1} \widetilde{(v_0)}_{,IK} \widetilde{Q}_{KJ} \quad , \tag{15}$$

where

$$\widetilde{(v_0)}_{,IK} = h_{mI} \ (v_0)_{,mn} \ h_{nJ} \tag{16}$$

are the second–order velocity derivatives in ray–centred coordinates.

7. First–order perturbations of the travel–time gradient

The first–order perturbations of the travel–time gradient expressed in ray–centred coordinates are

$$\widetilde{\tau}_{,I\alpha} = T^\perp_{J\alpha} \widetilde{Q}^{-1}_{JI} \quad , \tag{17}$$

where $\widetilde{Q}^{-1}_{JI}$ are the components of the matrix inverse to 2×2 matrix $\widetilde{Q}_{IJ}$ calculated by dynamic ray tracing (14) and (15). Here the covariant transform of the first–order perturbations of the travel–time gradient into ray parameters can be determined by numerical quadrature (Klimeš

2002, eq. 75)

$$T^{\perp}_{J\alpha}(\tau) = T^{\perp}_{J\alpha}(\tau^0) + \int_{\tau^0}^{\tau} \mathrm{d}\tau\, K^{\perp}_{J\alpha} \tag{18}$$

along the reference ray, with initial conditions $T^{\perp}_{J\alpha}(\tau^0)=0$ at the point source.

The ray–normal integration kernel for the perturbations of the travel–time gradient is (Klimeš 2002, eq. 80)

$$K^{\perp}_{J\alpha} = -(\widetilde{H}_{\alpha,I} + H_{\alpha}\widetilde{H}_{0,I})\widetilde{Q}_{IJ} - \widetilde{H}^{;I}_{\alpha}\widetilde{P}_{IJ} \quad . \tag{19}$$

The value of $\widetilde{\tau}_{,I\alpha}$ at the point source, where $T^{\perp}_{J\alpha}(\tau^0) = 0$ and $\widetilde{Q}_{IJ}(\tau^0) = 0$, can be obtained by the l'Hospital rule with respect to $\tau \to \tau^0+$,

$$\widetilde{\tau}_{,I\alpha}(\tau^0) = -(v_0)^{-2}\widetilde{H}^{;I}_{\alpha} \quad . \tag{20}$$

8. Second–order perturbations of travel time

The second–order perturbations of travel time can be determined by numerical quadrature (Klimeš 2002, eqs. 19 and 20)

$$\tau_{,\alpha\beta}(\tau) = \tau_{,\alpha\beta}(\tau^0) + \int_{\tau^0}^{\tau} \mathrm{d}\tau\, K_{\alpha\beta} \tag{21}$$

along the reference ray, with initial conditions $\tau_{,\alpha\beta}(\tau^0)=0$ at the point source.

The integration kernel for the second–order perturbations of travel time can be expressed as (Klimeš 2002, eq. 64)

$$K_{\alpha\beta} = -\widetilde{H}^{;I}_{\alpha}\widetilde{\tau}_{,I\beta} - \widetilde{H}^{;I}_{\beta}\widetilde{\tau}_{,I\alpha} - (v_0)^2\widetilde{\tau}_{,I\alpha}\widetilde{\tau}_{,I\beta} \quad . \tag{22}$$

The second–order perturbations of travel time calculated by quadrature (21) can be inserted into equation (11) for the travel–time errors due to the isotropic common ray approximation, and into equation (12) for the travel–time errors due to the anisotropic common ray approximation.

9. Numerical example

A vertically heterogeneous 1-D anisotropic model **QI** (model WA rotated by 45°) was provided by Pšenčík & Dellinger (2001). The density–normalized elastic moduli a_{ijkl} of the 1-D anisotropic model QI and of the reference isotropic model are interpolated linearly with depth. For their values at the surface (zero depth) and at the depth of 1 length unit refer to Bulant & Klimeš (2002a). To emphasize the effects of perturbations of travel time, new models with an increased degree of anisotropy have been derived from the QI model. The differences of the elastic moduli of model **QI2** from the elastic moduli of the reference isotropic model are exactly twice larger than the differences of model QI. Analogously, the differences of the elastic moduli of model **QI4** from the elastic moduli of the reference isotropic model are exactly 4 times larger than the differences of model QI. Note that the perturbation approach cannot be applied to model **QI8**, in which the differences of the elastic moduli from the elastic moduli of the reference isotropic model are exactly 8 times larger than the differences of model QI. Taylor expansion (10) with respect to the perturbations of the Hamiltonian does not seem to converge reasonably in model QI8.

The synthetic seismograms, corresponding to the vertical force at depth 0 km, are calculated at 29 receivers located in a vertical well located 1 km from the source. The source time function is the Gabor signal with reference frequency $f = 50$ Hz, slightly band–pass filtered by a cosine filter. The data for model QI may be found on the compact disk of Bucha, Bulant & Klimeš (2001). For comparison of the isotropic and anisotropic ray theory seismograms, coupling ray theory seismograms, and the anisotropic reflectivity calculations in model QI, and for a more detailed discussion and description of this model refer to Pšenčík & Dellinger (2001).

The coupling ray theory synthetic seismograms, corresponding to the anisotropic ray theory reference rays in models QI, QI2 and QI4, have been approximated by the second–order perturbation of travel time along isotropic rays. They are compared with the seismograms calculated by the isotropic common ray approximation of the coupling ray theory in Figure 1.

The individual terms in the second–order Taylor expansion (10) of the anisotropic ray theory travel times in the vicinity of isotropic common rays are displayed in Table 1. The differences between the second–order Taylor expansion (10) and the anisotropic ray theory travel times calculated by program ANRAY version 4.20 are also given. The quadratic terms (11) in Taylor expansion (10) represent the estimates of the errors due to the isotropic common ray (ICR) approximation of the anisotropic ray theory travel times. Also shown is estimate (12) of the errors due to the anisotropic common ray (ACR) approximation.

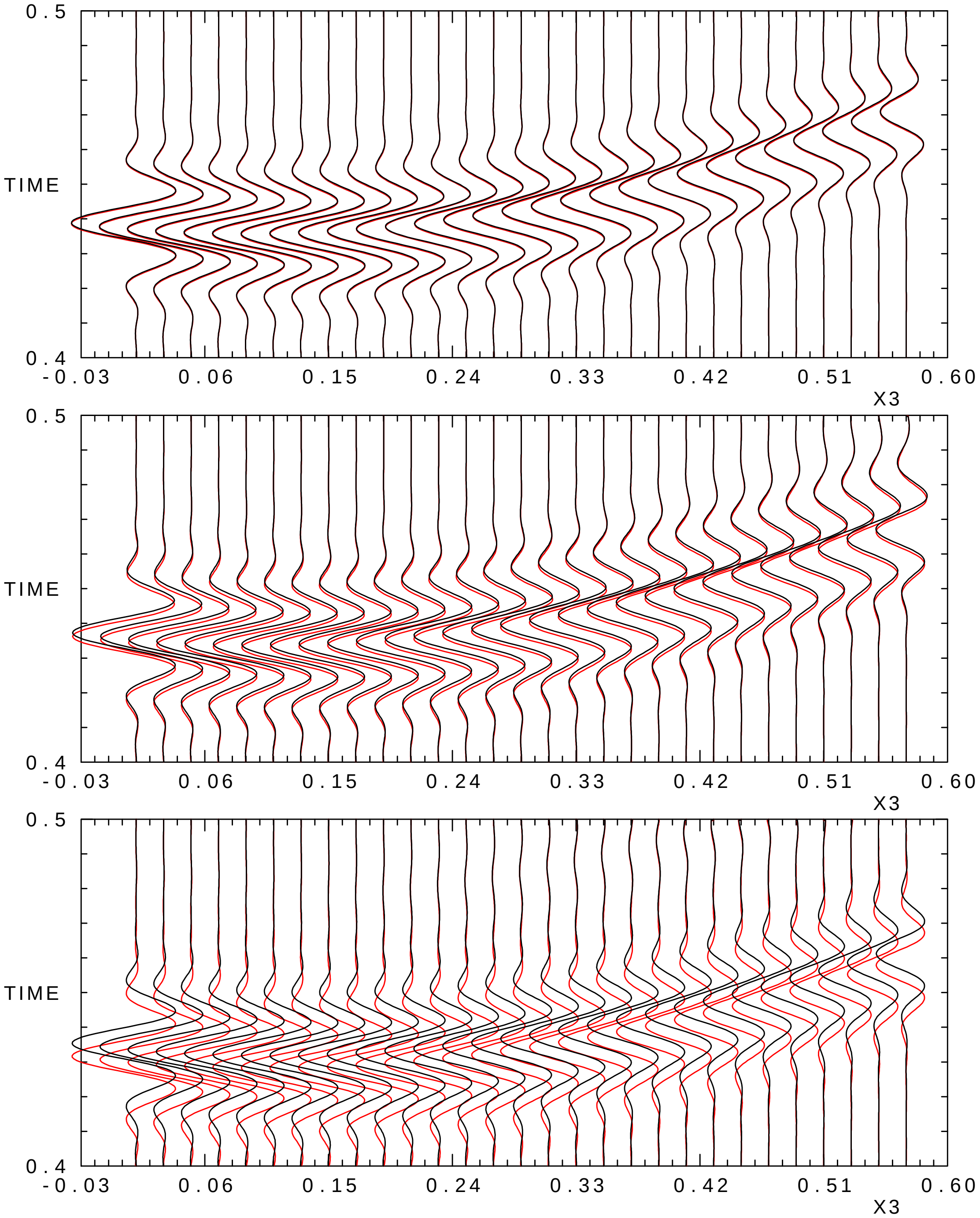

Figure 1. Vertical component of the coupling ray theory synthetic seismograms. From top to bottom: model QI, model QI2, model QI4. The *black line* corresponds to the *anisotropic reference rays*, simulated by the second–order perturbation of travel time along isotropic rays. The inaccuracy of this simulation is negligible in models QI and QI2, and roughly corresponds to the line thickness in model QI4 , see Table 1. The *red line* corresponds to the *isotropic common ray* approximation of the coupling ray theory. The differences due to the isotropic common ray approximation are mostly obscured in model QI, are small but already visible in model QI2, and are considerable in quite strongly anisotropic model QI4.

The accuracy of the anisotropic common ray approximation by Bakker (2002) in model QI2 would be even better than the accuracy of the isotropic common ray approximation in model QI, see Table 1. The first–order isotropic common ray approximation is considerably inaccurate in model QI4, see Figure 1 and Table 1. The inaccuracy of the second–order Taylor expansion (10) of travel time in model QI4 roughly corresponds to the line thickness in Figure 1. The first–order anisotropic common ray approximation by Bakker (2002) seems well applicable even in quite strongly anisotropic model QI4, and its accuracy is even better than the accuracy of the second–order Taylor expansion (10) from the isotropic common ray, see Table 1.

	ICR time	ICR linear terms		ICR quadratic terms		ICR remaining terms		ACR q.terms
QI	0.440985	-0.002392	0.003983	0.000258	0.000000	0.000000	0.000006	0.000068
QI	0.475198	-0.004520	0.004595	0.000244	0.000001	0.000021	0.000008	0.000075
QI2	0.440985	-0.004747	0.011604	0.001001	0.000000	-0.000013	0.000002	0.000242
QI2	0.475198	-0.008912	0.012764	0.000932	0.000000	0.000088	0.000006	0.000215
QI4	0.440985	-0.009344	0.041578	0.003755	0.000504	0.000018	-0.000141	0.000376
QI4	0.475198	-0.017335	0.042241	0.003358	0.001209	0.000499	-0.000200	0.000134

Table 1. First–order and second–order terms in the common ray approximations of travel time at the outermost receivers in models QI, QI2 and QI4. The *ICR time* is the reference travel time τ along the isotropic common ray. The *ICR linear terms* are the linear terms $\tau_{,1}$ and $\tau_{,2}$ in Taylor expansion (10) of the aniso0.tropic ray theory travel times in the vicinity of the isotropic common ray, and represent the travel–time corrections considered in the isotropic common ray approximation of the coupling ray theory. The *ICR quadratic terms* stand for second–order terms (11) in Taylor expansion (10) of travel time, and represent the estimates of the errors due to the isotropic common ray approximation of the aniso0.tropic ray theory travel times. The *ICR remaining terms* stand for the difference between the exact aniso0.tropic ray theory travel times calculated by program ANRAY version 4.20 (Pšenčík 1998b) and the second–order Taylor expansion (10), in order to illustrate the reliability of the error estimates. The *ACR quadratic terms* stand for the estimate (12) of equal quadratic terms in Taylor expansion of the aniso0.tropic ray theory travel times in the vicinity of the aniso0.tropic common ray, and represent the estimate of the error due the aniso0.tropic common ray approximation (Bakker 2002) of the aniso0.tropic ray theory travel times.

Although we have successfully applied the second–order perturbations of travel time to the estimation of anisotropic ray theory travel times in these simple 1-D models with constant gradients of the density–normalized elastic moduli, we cannot recommend approximation of travel time using the second–order perturbations in more complex models, because the second–order perturbations may be infinitely large in the vicinity of caustics. The second–order perturbations of travel time should be used especially for estimating and controlling the accuracy.

10. Conclusions

When using any kind of the common ray approximation of the coupling ray theory, the travel–time errors due to the applied common ray approximation should be evaluated. The travel–time errors due to the common ray approximations can be calculated using the equations proposed in this paper. If the errors of the isotropic common ray approximation exceed an acceptable limit, we can immediately decide whether the anisotropic common ray approximation (Bakker 2002) would be sufficiently accurate, or whether the anisotropic ray theory rays should be traced as reference rays for the coupling ray theory. The accuracy of the anisotropic common ray approximation by Bakker (2002) can be studied without tracing the anisotropic common rays. The numerical results suggest that the anisotropic common ray approximation by Bakker (2002) is worth coding and applying.

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