ERRORS DUE TO THE ANISOTROPIC-COMMON-RAY APPROXIMATION OF THE COUPLING RAY THEORY

L. KLIMEŠ AND P. BULANT

Department of Geophysics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Praha 2, Czech Republic
(http://sw3d.mff.cuni.cz/staff/klimes.htm, http://sw3d.mff.cuni.cz/staff/bulant.htm)

Received: October 7, 2005; Revised: February 20, 2006; Accepted: April 9, 2006

ABSTRACT

The common–ray approximation eliminates problems with ray tracing through S–wave singularities and also considerably simplifies the numerical algorithm of the coupling ray theory for S waves, but may introduce errors in travel times due to the perturbation from the common reference ray. 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 errors due to the common–ray approximation applied.

The anisotropic–common–ray approximation of the coupling ray theory is more accurate than the isotropic–common–ray approximation. We derive the equations for estimating the travel–time errors due to the anisotropic–common–ray (and also isotropic–common–ray) approximation of the coupling ray theory. The errors of the common–ray approximations are calculated along the anisotropic common rays in smooth velocity models without interfaces. The derivation is based on the general equations for the second–order perturbations of travel time.

Key words: coupling ray theory, common–ray approximation, travel time, perturbation theory, seismic anisotropy, heterogeneous media

1. INTRODUCTION

There are two different high–frequency asymptotic ray theories: the *isotropic ray theory* based on the assumption of equal velocities of both S waves, and the *anisotropic ray theory* assuming both S waves strictly decoupled. In the isotropic ray theory, the S–wave polarization vectors do not rotate about the ray, whereas in the anisotropic ray theory they coincide with the eigenvectors of the Christoffel matrix which may rotate rapidly about the ray. *Thomson et al. (1992)* demonstrated analytically that the high–frequency asymptotic error of the anisotropic–ray–theory wavefield is inversely proportional to the second or higher root of the frequency if a ray passes through the point of equal S–wave eigenvalues of the Christoffel matrix even in an otherwise strongly anisotropic medium.

In "weakly anisotropic" models, at moderate frequencies, the S–wave polarization tends to remain 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. This behaviour of the S–wave polarization is described by the *coupling ray theory* proposed by *Coates and Chapman (1990)*. The frequency–dependent coupling ray theory is the generalization of both the zero–order isotropic and anisotropic ray theories and provides continuous transition between them. The coupling ray theory is applicable to S waves at all degrees of anisotropy, from isotropic to considerably anisotropic velocity models. The numerical algorithm for calculating the frequency–dependent complex–valued S–wave polarization vectors of the coupling ray theory has been designed by *Bulant and Klimeš (2002)*.

There are many commonly used *quasi–isotropic approximations* of the coupling ray theory (e.g., *Pšenčík, 1998*), which diminish the accuracy of the coupling ray theory both with increasing frequency and increasing degree of anisotropy. Refer to *Bulant and Klimeš (2002, 2004)* and to *Klimeš and Bulant (2004)* for the description of individual quasi–isotropic approximations and for the examples of their impact on synthetic seismograms. Most of these quasi–isotropic approximations can be avoided with minimal effort except for the *common–ray approximation* for S waves.

In the common–ray approximation, only one reference ray is traced for both anisotropic–ray–theory S waves, and both S–wave anisotropic–ray–theory travel times are approximated by the perturbation expansion from the common reference ray. Whereas tracing the continuous system of anisotropic–ray–theory rays may be very difficult in the vicinity of an S–wave singularity at which the S–wave slowness surfaces coincide (*Vavryčuk, 2003*), this problem does not occur in the common–ray approximation. The common–ray approximation thus eliminates problems with ray tracing through S–wave singularities and also considerably simplifies 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 travel–time errors due to the common–ray approximation, and then the related error of the wavefield.

In the common–ray approximation, the S–wave travel times are usually approximated by the first–order perturbation expansion from the common reference ray. The errors of S–wave travel times may then be approximated by the second–order terms in the perturbation expansion. Note that the perturbation expansion is the Taylor expansion with respect to the perturbation parameters, see (19), which parametrize the Hamiltonian, see (18). We refer here to the partial derivatives with respect to the perturbation parameters as perturbation derivatives, in order to distinguish them from the partial derivatives with respect to the spatial coordinates.

The common reference rays have routinely been represented by the *isotropic common rays* calculated in the isotropic reference model, but they would better be represented by the *anisotropic common rays*. The anisotropic common rays are traced in the anisotropic model, using the averaged Hamiltonian of both anisotropic–ray–theory S waves (*Bakker, 2002*). The algorithm of the dynamic ray tracing corresponding to the anisotropic common rays was proposed by *Klimeš (2006b)*. The numerical results of *Klimeš and Bulant (2004)* and *Bulant and Klimeš (2006)* demonstrate that the *anisotropic–common–ray approximation* is considerably more accurate than the *isotropic–common–ray approximation*. For a more detailed description of the common–ray approximations of the coupling ray theory refer to Section 2. In Sections 2 and 4, the information of sections 2.1 and 2.2 by *Klimeš and Bulant (2004)* is reviewed for the reader's convenience.

Klimeš and Bulant (2004) derived the equations for estimating the travel–time errors due to the isotropic–common–ray and anisotropic–common–ray approximations by numerical quadrature along the *isotropic common rays* in smooth velocity models without interfaces. The accuracy of the isotropic–common–ray approximation can thus be checked routinely. In addition, the accuracy of the anisotropic–common–ray approximation can be studied approximately along isotropic common rays, without tracing the anisotropic common rays. If the error of the isotropic–common–ray approximation exceeds an acceptable limit, we can decide immediately whether the anisotropic–common–ray approximation would be sufficiently accurate, or whether the anisotropic–ray–theory rays should be traced as reference rays for the coupling ray theory.

In this paper, we propose the equations for estimating the travel–time errors due to the anisotropic–common–ray (and also isotropic–common–ray) approximation by numerical quadrature along the *anisotropic common rays* in smooth velocity models without interfaces. The derivation for estimating the errors along the anisotropic common rays is based on the general equations for the second–order perturbations of travel time by *Klimeš (2002)*, and is analogous to the derivation by *Klimeš and Bulant (2004)* for estimating the errors along the isotropic common rays. The equations for estimating the travel–time errors due to the common–ray approximations of the coupling ray theory for S waves are derived in a form suitable for dynamic ray tracing in ray–centred coordinates attached to the anisotropic common rays. The accuracy of the anisotropic–common–ray approximation can thus be checked routinely using the equations derived in this paper in Sections 5 to 10.

Bulant and Klimeš (2006) numerically tested the derived equations in three smooth 1–D velocity models of differing degree of anisotropy, and compared the travel–time errors due to the anisotropic–common–ray approximation of the coupling ray theory with the errors due to the isotropic–common–ray approximation. The errors of the anisotropic–common–ray approximation are considerably smaller than the errors of the isotropic–common–ray approximation as expected.

For additional information, including papers, computer codes and data, refer to the consortium research project "Seismic Waves in Complex 3–D Structures" ("http://sw3d.mff.cuni.cz").

2. SELECTION OF THE REFERENCE RAY

The isotropic ray theory is always the limiting case of the coupling ray theory for decreasing anisotropy at a fixed frequency. On the other hand, the high–frequency limit of the coupling ray theory at a fixed anisotropy depends 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. The reference ray should be "close to the ray of the coupled S wave under study". Unfortunately, this is but a rough statement, because the ray of the coupled S wave has not been defined yet.

From the point of view of the high–frequency asymptotic validity, the frequency–independent reference ray is best represented by the *anisotropic–ray–theory reference ray*, provided we choose the initial condition for the polarization vector in the coupling equation given by the eigenvector of the Christoffel matrix corresponding to the reference ray. The anisotropic–ray–theory travel time corresponding to the selected polarization is then exact, and only the difference between the two anisotropic–ray–theory S–wave travel times 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 converges 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, although the differences may be small at the finite frequencies under consideration. Note that the anisotropic–ray–theory reference ray can be traced only if the eigenvectors of the Christoffel matrix vary continuously along the whole ray (*Vavryčuk, 2001*).

In the *anisotropic–common–ray approximation*, the common reference ray is traced using the averaged Hamiltonian of both anisotropic–ray–theory S waves (*Bakker, 2002*; *Klimeš, 2006b*). This is probably the best common–ray approximation. The errors due to the anisotropic–common–ray approximation of the coupling ray theory are usually considerably smaller than the errors due to the routinely used isotropic–common–ray approximation of the coupling ray theory (*Klimeš and Bulant, 2004; Bulant and Klimeš, 2006*).

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 differing accuracies.

3. COUPLING RAY THEORY

For the derivation of the coupling ray theory refer to *Coates and Chapman (1990)* and to *Červený (2001)*. For the description of the numerical algorithm of the coupling ray theory refer to *Bulant and Klimeš (2002)*. The numerical algorithm of the coupling ray theory by *Bulant and Klimeš (2002)* is independent of the reference ray. The algorithm is thus applicable to isotropic common rays, to anisotropic common rays, and also to anisotropic–ray–theory reference rays.

The algorithms of anisotropic common S–wave ray tracing in smooth anisotropic models without interfaces and of the corresponding dynamic ray tracing in ray–centred coordinates are described by *Klimeš (2006a, 2006b)*. We thus have all equations necessary for the anisotropic–common–ray approximation of the coupling ray theory.

Here we shall concentrate only on estimating the travel–time errors due to the anisotropic–common–ray (and also isotropic–common–ray) approximation by numerical quadrature along the anisotropic common rays. The estimates are based on the equations for the second–order perturbation derivatives of travel time derived by *Klimeš (2002)*.

4. TRAVEL TIMES IN THE COUPLING RAY THEORY

Let $a_{ijkl} = a_{ijkl}(x_m)$ be the density–normalized elastic moduli describing a *smooth anisotropic model*, in which the *anisotropic common rays* are traced using the averaged Hamiltonian of both anisotropic–ray–theory S waves. For completeness, we also introduce S–wave velocity $v_0 = v_0(x_m)$ in the smooth reference isotropic model in which the isotropic common rays could be traced.

Assume a phase–space *reference ray*, parametrized by reference travel time τ, with reference slowness vectors $p_i(\tau)$ known at all its points $x_j(\tau)$. In this section, the reference ray is general, including the anisotropic common ray and isotropic common ray as special cases. Using the reference slowness vectors, we can calculate the 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 or the perturbation parameters. Assume that eigenvectors $g_{i1}(\tau)$ and $g_{i2}(\tau)$ correspond to the S waves. For application of the coupling ray theory, the eigenvectors should vary continuously along the reference ray (*Bulant and Klimeš, 2002*). This condition is not required in regions where the two S–wave eigenvalues of the Christoffel matrix are approximately equal.

Let us denote by $\tau_\alpha(\tau)$ the anisotropic–ray–theory travel time corresponding to the selected eigenvector $g_{i\alpha}(\tau)$ of the Christoffel matrix. 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 and Klimeš (2002)*, would become exact for a reference ray following the path of the respective anisotropic–ray–theory ray. Travel–time approximation (2) can be derived as the first–order part of perturbation expansion (19), corresponding to Hamiltonian

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

see Section 7. Here $G_\alpha(x_m, p_n)$ is the eigenvalue of Christoffel matrix (1), corresponding to eigenvector $g_{i\alpha}$. Hamiltonian (3) is a homogeneous function of the minus first degree with respect to the slowness vector.

5. REFERENCE HAMILTONIAN, ANISOTROPIC–RAY–THEORY HAMILTONIANS, AND ISOTROPIC–RAY–THEORY HAMILTONIAN

We denote by $H_0(x_m, p_n)$ the *reference Hamiltonian* used to trace the reference ray.

For the anisotropic common ray, *Klimeš (2006b)* assumed the reference Hamiltonian to be equal to the averaged Hamiltonian

$$\overline{H}_0(x_m, p_n) = \tfrac{1}{2}\left\{\tfrac{1}{2}\{[G_1(x_m, p_n)]^{\frac{N}{2}} + [G_2(x_m, p_n)]^{\frac{N}{2}}\}\right\}^{\frac{2}{N}} \tag{4}$$

of both S waves (*Klimeš, 2006b, eqs. 28 and 36*), where constant N specifies the way of averaging. Note that *Bakker (2002)* considered $N = 2$. Hamiltonian (4) is a homogeneous function of the second degree with respect to the slowness vector. The value of Hamiltonian (4) along the reference ray is $\overline{H}_0(x_m, p_n) = \frac{1}{2}$.

The first–order phase–space derivatives of Hamiltonian (4) are determined by equations (29) and (37) of *Klimeš (2006b)*. The second–order phase–space derivatives of Hamiltonian (4) are determined by equations (31) and (38) of *Klimeš (2006b)*.

Since the equations for the perturbation derivatives of travel time were derived by *Klimeš (2002)* on the condition that the Hamiltonian has an equal value for all orthonomic systems of rays under consideration, reference Hamiltonian $H_0(x_m, p_n)$ must be a homogeneous function of the same degree with respect to the slowness vector as Hamiltonian (3). We thus select reference Hamiltonian

$$H_0(x_m, p_n) = -[2\overline{H}_0(x_m, p_n)]^{-\frac{1}{2}} \quad , \tag{5}$$

which is a homogeneous function of the minus first degree with respect to the slowness vector, and which yields equal orthonomic systems of rays as Hamiltonian (4). Along the reference ray, the value of Hamiltonian (5) is

$$H_0(x_m, p_n) = -1 \quad , \tag{6}$$

the values of the first–order partial derivatives with respect to the spatial coordinates (denoted by Roman subscripts following a comma) of Hamiltonian (5) are

$$\boxed{H_{0,i} = \overline{H}_{0,i} \quad , \qquad (7)}$$

the values of the first–order partial derivatives with respect to the components of the slowness vector (denoted by Roman superscripts following a comma) of Hamiltonian (5) are

$$\boxed{H_0^{,i} = \overline{H}_0^{,i} \quad , \qquad (8)}$$

the values of the second–order partial derivatives of Hamiltonian (5) with respect to the spatial coordinates are

$$\boxed{H_{0,ij} = \overline{H}_{0,ij} - 3\overline{H}_{0,i}\overline{H}_{0,j} \quad ,} \tag{9}$$

and the values of the second–order partial derivatives of Hamiltonian (5) with respect to the components of the slowness vector are

$$\boxed{H_0^{;ij} = \overline{H}_0^{;ij} - 3\overline{H}_0^{;i}\overline{H}_0^{;j} \quad .} \tag{10}$$

The value of Hamiltonian (3), corresponding to unit S–wave eigenvector $g_{i\alpha}$, $\alpha = 1, 2$ of the Christoffel matrix, at the reference ray, is

$$\boxed{H_\alpha = -(a_{ijkl}g_{i\alpha}p_j g_{k\alpha}p_l)^{-\frac{1}{2}} \quad .} \tag{11}$$

The partial derivatives of Hamiltonian (11) with respect to the spatial coordinates are

$$\boxed{H_{\alpha,i} = -\tfrac{1}{2}(H_\alpha)^3 a_{mjkl,i}g_{m\alpha}p_j g_{k\alpha}p_l \quad .} \tag{12}$$

The partial derivatives of Hamiltonian (11) with respect to the components of the slowness vector are

$$\boxed{H_\alpha^{;i} = -(H_\alpha)^3 a_{mikl}g_{m\alpha}g_{k\alpha}p_l \quad .} \tag{13}$$

The values of phase–space derivatives (12) and (13) are calculated at the reference ray in this paper. Partial derivatives (13) satisfy Euler's relation

$$H_\alpha^{;i}p_i = -H_\alpha \tag{14}$$

for a homogeneous function of degree -1 with respect to p_i.

The quantities enclosed above in boxes are necessary for estimating the errors due to the anisotropic–common–ray approximation of the coupling ray theory.

To be able to calculate the travel–time perturbations from the anisotropic common ray towards the isotropic–ray–theory ray, we also introduce homogeneous Hamiltonian

$$H_3(x_m, p_n) = -[v_0(x_m)]^{-1}(p_ip_i)^{-\frac{1}{2}} \tag{15}$$

for the reference isotropic medium. Hamiltonian (15) is a homogeneous function of the minus first degree with respect to the slowness vector. The partial derivatives of Hamiltonian (15) with respect to spatial coordinates x_i are

$$H_{3,i} = v_{0,i}\,(v_0)^{-2}(p_kp_k)^{-\frac{1}{2}} \quad . \tag{16}$$

The partial derivatives of Hamiltonian (15) with respect to the components of the slowness vector are

$$H_3^{;i} = (v_0)^{-1}(p_kp_k)^{-\frac{3}{2}}p_i \quad . \tag{17}$$

6. PARAMETRIC SYSTEM OF THE HAMILTONIANS AND ERRORS DUE TO THE COMMON–RAY APPROXIMATIONS

We consider the parametric set $H = H(x_m, p_n, f_\alpha)$ of Hamiltonians parametrized by f_α,

$$H(x_m, p_n, f_\alpha) = H_0(x_m, p_n) + \sum_\alpha [H_\alpha(x_m, p_n) - H_0(x_m, p_n)]\, f_\alpha \quad , \tag{18}$$

where $\alpha = 1, 2$ for perturbations towards the anisotropic–ray–theory rays. If we are also interested in the perturbations towards a reference isotropic model, $\alpha = 1, 2, 3$. Parameters f_α are called *perturbation parameters* (*Baumgärtel, 1985*; *Murdock, 1999*; *Klimeš and Bulant, 2004*) or model parameters (*Tarantola, 1987*; *Klimeš, 2002*). Parametric system (18) of the Hamiltonians then generates parametric system $\tau(x_m, f_\alpha)$ of the travel–time fields corresponding to the individual Hamiltonians $H(x_m, p_n, f_\alpha)$.

We obtain the reference Hamiltonian for $(f_1, f_2, f_3) = (0, 0, 0)$, the Hamiltonian corresponding to the first anisotropic–ray–theory S wave for $(f_1, f_2, f_3) = (1, 0, 0)$, the Hamiltonian corresponding to the second anisotropic–ray–theory S wave for $(f_1, f_2, f_3) = (0, 1, 0)$, and the Hamiltonian corresponding to the isotropic–ray–theory ray traced in the reference isotropic model for $(f_1, f_2, f_3) = (0, 0, 1)$.

The Taylor expansion with respect to perturbation parameters f_α is called here the *perturbation expansion.* The second–order perturbation expansion of travel time is

$$\tau(x_m, f_\alpha) \approx \tau(x_m) + \sum_\alpha \tau_{,\alpha}(x_m) f_\alpha + \tfrac{1}{2} \sum_\alpha \sum_\beta \tau_{,\alpha\beta}(x_m) f_\alpha f_\beta \quad , \tag{19}$$

where the Greek subscripts following a comma denote partial derivatives with respect to perturbation parameters f_α, hereinafter called *perturbation derivatives.* Note that *Klimeš (2002)* refers to the perturbation derivatives briefly as the "perturbations". Here, travel time $\tau(x_m)$ and its perturbation derivatives $\tau_{,\alpha}(x_m)$, $\tau_{,\alpha\beta}(x_m)$, with arguments f_α omitted, correspond to the reference system of rays $(f_1, f_2, f_3) = (0, 0, 0)$.

Travel–time approximation (2) corresponds to the first–order part of perturbation expansion (19), see Section 7. The error of travel–time approximation (2) may thus be approximated by the quadratic term in perturbation expansion (19) with Hamiltonians (18).

We may now express the estimates of the travel–time errors due to the *anisotropic–common–ray* (ACR) *approximation* (*Bakker, 2002*; *Klimeš, 2006b*) of anisotropic travel times in terms of the second–order perturbation derivatives of travel time. The errors of travel–time approximation (2) from anisotropic common ray $(f_1, f_2, f_3) = (0, 0, 0)$ to anisotropic–ray–theory ray $(f_1, f_2, f_3) = (1, 0, 0)$ and to anisotropic–ray–theory ray $(f_1, f_2, f_3) = (0, 1, 0)$ are approximately

$$\boxed{\delta\tau_\alpha^{\mathrm{ACR}} = \frac{\tau_{,\alpha\alpha}}{2} \quad ,} \tag{20}$$

where $\alpha=1,2$. Equation (20) with $\alpha=3$ analogously yields the second–order term in the perturbation expansion from the anisotropic common ray to the isotropic–ray–theory ray traced in the reference isotropic model.

We may also use the second–order perturbation derivatives of travel time, calculated along the anisotropic common ray, to estimate the accuracy of the *isotropic–common–ray* (ICR) *approximation*. The estimates of errors of travel–time approximation (2) from isotropic common ray $(f_1, f_2, f_3) = (0, 0, 1)$ to anisotropic–ray–theory ray $(f_1, f_2, f_3) = (1, 0, 0)$ and to anisotropic–ray–theory ray $(f_1, f_2, f_3) = (0, 1, 0)$ are

$$\delta\tau_\alpha^{\mathrm{ICR}} = \tfrac{1}{2}\tau_{,\alpha\alpha} - \tau_{,\alpha 3} + \tfrac{1}{2}\tau_{,33} \quad , \tag{21}$$

where $\alpha = 1, 2$. Error estimates (21) represent the contributions of the quadratic terms in perturbation expansion (19) from the isotropic common ray to the anisotropic–ray–theory S–wave rays.

To calculate the first–order and second–order perturbation derivatives $\tau_{,\alpha}$ and $\tau_{,\alpha\beta}$ of travel time, we need the first–order and second–order phase–space and perturbation derivatives of the Hamiltonian. The phase–space and perturbation derivatives of Hamiltonian (18) in the reference model $f_\alpha=0$ are

$$H_{,i} = H_{0,i} \quad , \tag{22}$$

$$H^{,i} = H_0^{,i} \quad , \tag{23}$$

$$H_{,ij} = H_{0,ij} \quad , \tag{24}$$

$$H^{,ij} = H_0^{,ij} \quad , \tag{25}$$

$$H_{,\alpha} = H_\alpha - H_0 \quad , \tag{26}$$

$$H_{,i\alpha} = H_{\alpha,i} - H_{0,i} \quad , \tag{27}$$

$$H^{,i}_{,\alpha} = H^{,i}_\alpha - H^{,i}_0 \quad , \tag{28}$$

$$H_{,\alpha\beta} = 0 \quad , \tag{29}$$

where the Greek subscripts following a comma denote the partial derivatives with respect to perturbation parameters f_α, analogously as for travel time.

7. FIRST–ORDER PERTURBATION EXPANSION OF TRAVEL TIME

The first–order perturbation derivatives of travel time can be determined by numerical quadrature (*Klimeš, 2002, eqs. 19 and 25*)

$$\tau_{,\alpha}(\tau) = \tau_{,\alpha}(\tau^0) - \int_{\tau^0}^{\tau} \mathrm{d}\tau \; H_{,\alpha} \tag{30}$$

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

Inserting (26) for $H_{,\alpha}$ into equation (30) and considering (6), we obtain

$$\tau(\tau) + \tau_{,\alpha}(\tau) = \tau(\tau^0) + \tau_{,\alpha}(\tau^0) - \int_{\tau^0}^{\tau} \mathrm{d}\tau \; H_\alpha \quad . \tag{31}$$

This is the first–order part of perturbation expansion (19) of travel time from anisotropic common ray $(f_1, f_2, f_3)=(0,0,0)$ to anisotropic–ray–theory rays $(f_1, f_2, f_3)=(1,0,0)$ and $(f_1, f_2, f_3)=(0,1,0)$, or to isotropic common ray $(f_1, f_2, f_3)=(0,0,1)$.

Equation (31) with (11) for $\alpha = 1,2$ yields travel–time approximation (2) used in the coupling ray theory. Equation (31) with (15) for $\alpha = 3$ represents the first–order perturbation expansion from the anisotropic common ray to the isotropic common ray.

8. DYNAMIC RAY TRACING AND RAY–CENTRED COORDINATES

We define the matrices of the partial derivatives of spatial coordinates x_i and of the slowness–vector components $p_i = \tau_{,i}$ with respect to 3 *ray coordinates*: ray take–off parameters γ_1, γ_2, and independent parameter $\gamma_3 = \tau$ along rays,

$$Q_{ia} = \frac{\partial x_i}{\partial \gamma_a} \quad , \qquad P_{ia} = \frac{\partial \tau_{,i}}{\partial \gamma_a} \quad . \tag{32}$$

Matrices Q_{ia} and P_{ia} can be calculated by numerically solving a set of linear ordinary differential equations called the *dynamic ray tracing equations* (*Červený, 1972*). Matrices Q_{ia} and P_{ia} describe, by definition, the properties of the orthonomic system of rays corresponding to the travel time under consideration. They may be expressed in terms of their initial values and the paraxial ray propagator matrix (*Červený, 2001*).

The second–order spatial derivatives $\tau_{,ij}$ of travel time can be expressed in terms of matrices Q_{ia} and P_{ia}. Equation

$$P_{ia} = \tau_{,ij}\, Q_{ja} \tag{33}$$

is a direct consequence of the above definitions (32).

Let us denote by h^i_1, h^i_2, h^i_3 the contravariant basis vectors, and by $\hat{h}_{i1}, \hat{h}_{i2}, \hat{h}_{i3}$ the covariant basis vectors of the *ray–centred coordinate system*. The basis vectors of the ray–centred coordinate system are calculated along the reference ray. The first two contravariant basis vectors h^i_M of the ray–centred coordinate system are tangent to the wavefront, the third contravariant basis vector $h^i_3 = H^{\,i}_0$ is tangent to the ray. The first two covariant basis vectors $\hat{h}_{iM}$ of the ray–centred coordinate system are perpendicular to the ray, the third covariant basis vector $\hat{h}_{i3} = p_i$ is perpendicular to the wavefront. The contravariant basis vectors and covariant basis vectors are mutually biorthonormal,

$$h^i_a \hat{h}_{ib} = \delta_{ab} \quad . \tag{34}$$

The equations for calculating the basis vectors of the ray–centred coordinate system can be found, e.g., in *Klimeš (2006a)*.

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

$$\widetilde{Q}_{ia} = \hat{h}_{mi} Q_{ma} \quad , \tag{35}$$

$$\widetilde{P}_{ia} = h_i^m P_{ma} \quad , \tag{36}$$

$$\widetilde{\tau}_{,ij} = h_i^m \tau_{,mn} h_j^n \quad , \tag{37}$$

$$\widetilde{\tau}_{,i\alpha} = h_i^m \tau_{,m\alpha} \quad , \tag{38}$$

$$\boxed{\begin{aligned} \widetilde{H}_{0,i} &= H_{0,m} h_i^m \quad , & (39)\\ \widetilde{H}_{0,ij} &= H_{0,mn} h_i^m h_j^n \quad , & (40)\\ \widetilde{H}_0^{;ij} &= H_0^{;mn} \hat{h}_{mi} \hat{h}_{nj} \quad , & (41)\\ \widetilde{H}_{\alpha,i} &= H_{\alpha,m} h_i^m \quad , & (42)\\ \widetilde{H}_\alpha^{;i} &= H_\alpha^{;m} \hat{h}_{mi} \quad . & (43) \end{aligned}}$$

Since we consider matrices Q_{ia} and P_{ia} defined for $\gamma_3 = \tau$,

$$\widetilde{Q}_{3J} = 0 \quad . \tag{44}$$

The 2×2 submatrices $\widetilde{Q}_{IJ}$ and $\widetilde{P}_{IJ}$ of matrices (35) and (36) are usually calculated by the *dynamic ray tracing equations in ray–centred coordinates* (*Klimeš, 1994, eq. 60*)

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \widetilde{Q}_{IJ} = \widetilde{\widetilde{H}}{}_{0,K}^{;I} \, \widetilde{Q}_{KJ} + \widetilde{H}_0^{;IK} \, \widetilde{P}_{KJ} \quad , \tag{45}$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \widetilde{P}_{IJ} = -\widetilde{\widetilde{H}}_{0,IK} \, \widetilde{Q}_{KJ} - \widetilde{\widetilde{H}}{}_{0,I}^{;K} \, \widetilde{P}_{KJ} \quad . \tag{46}$$

For the second–order phase–space derivatives

$$\widetilde{\widetilde{H}}_{0,IK} = \widetilde{H}_{0,IK} + 2\widetilde{H}_{0,I} \widetilde{H}_{0,K} \quad , \tag{47}$$

$\widetilde{\widetilde{H}}{}_{0,K}^{;I}$ and $\widetilde{\widetilde{H}}{}_0^{;IK} = \widetilde{H}_0^{;IK}$ of the reference Hamiltonian in ray–centred coordinates refer to *Klimeš (1994, eqs. 51a, 51b, 51c)* or to *Klimeš (2006b, eqs. 60–62)*.

We shall thus express the equations for estimating the travel–time errors due to the common–ray approximations of the coupling ray theory in terms of the 2×2 matrices $\widetilde{Q}_{IJ}$ and $\widetilde{P}_{IJ}$ in ray–centred coordinates.

9. FIRST–ORDER PERTURBATION DERIVATIVES OF THE TRAVEL–TIME GRADIENT

To calculate the second–order perturbation derivatives of travel time, we need to know at least the ray–normal projection

$$\tau_{,i\alpha}^{\perp} = E_i^{\perp j} \tau_{,j\alpha} \tag{48}$$

of the first–order perturbation derivatives $\tau_{,i\alpha}$ of the travel–time gradient (*Klimeš, 2002, eqs. 54 and 55*). The ray–normal projection matrix $E_i^{\perp j}$ can be expressed in terms of the first two basis vectors of the ray–centred coordinate system,

$$E_i^{\perp j} = \hat{h}_{iM} h_M^j \quad . \tag{49}$$

The covariant transform (*Klimeš, 2002, eq. 69*)

$$T^{\perp}_{J\alpha} = \tau^{\perp}_{,i\alpha}\, Q_{iJ} \tag{50}$$

of ray–normal derivatives (48) into ray coordinates can be determined by numerical quadrature (*Klimeš, 2002, eq. 75*)

$$\boxed{T^{\perp}_{J\alpha}(\tau) = T^{\perp}_{J\alpha}(\tau^0) + \int_{\tau^0}^{\tau} \mathrm{d}\tau\, K^{\perp}_{i\alpha} Q_{iJ}} \tag{51}$$

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

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

$$K^{\perp}_{i\alpha} = E^{\perp}_{i}{}^{a} \left(-H_{,a\alpha} + H_{,a}\, H_{,\alpha}^{;r}\, p_r\right) - H_{,\alpha}^{;r}\, \tau^{\perp}_{,ri} \quad , \tag{52}$$

where

$$\tau^{\perp}_{,ij} = E^{\perp}_{i}{}^{a} E^{\perp}_{j}{}^{b} \tau_{,ab} \tag{53}$$

is the ray–normal projection of the second–order spatial derivatives $\tau_{,ij}$ of travel time.

Inserting equations (22), (27), (28) with (14) and (34), and (53) into (52), we arrive at

$$K^{\perp}_{i\alpha} = -E^{\perp}_{i}{}^{a} \left(H_{\alpha,a} + H_{\alpha} H_{0,a}\right) - H_{\alpha}^{;r} E^{\perp}_{r}{}^{a} \tau_{,ab} E^{\perp}_{i}{}^{b} \quad . \tag{54}$$

Multiplying equation (54) by the first two columns Q_{iJ} of the matrix of geometrical spreading, inserting equation (49), and considering transforms (35), (36), (37) and relations (33), (34) and (44), we arrive at

$$\boxed{K^{\perp}_{i\alpha} Q_{iJ} = -(\widetilde{H}_{\alpha,I} + H_{\alpha} \widetilde{H}_{0,I})\, \widetilde{Q}_{IJ} - \widetilde{H}_{\alpha}^{;I}\, \widetilde{P}_{IJ} \quad ,} \tag{55}$$

where $\widetilde{Q}_{IJ}$ and $\widetilde{P}_{IJ}$ are the 2×2 submatrices of matrices (35) and (36). The 2×2 matrices $\widetilde{Q}_{IJ}$ and $\widetilde{P}_{IJ}$ are usually calculated by the dynamic ray tracing equations (45) and (46) in ray–centred coordinates.

Inserting equations (48) and (49) into (50) while considering transforms (35) and (38), we arrive at

$$T^{\perp}_{J\alpha} = \widetilde{\tau}_{,I\alpha}\, \widetilde{Q}_{IJ} \quad . \tag{56}$$

The first–order perturbation derivatives of the travel–time gradient expressed in ray–centred coordinates are then

$$\boxed{\widetilde{\tau}_{,I\alpha} = T^{\perp}_{J\alpha} \widetilde{Q}^{-1}_{JI} \quad ,} \tag{57}$$

where $\widetilde{Q}^{-1}_{JI}$ are the components of the matrix inverse to 2×2 matrix $\widetilde{Q}_{IJ}$ calculated by dynamic ray tracing (45) and (46) in ray–centred coordinates.

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 from equation (57) by the l'Hospital rule with respect to $\tau \to \tau^0 +$. Equation (45) and derivative (55) of equation (51) with $\widetilde{Q}_{IJ} = 0$ then yield

$$\boxed{\widetilde{\tau}_{,I\alpha}(\tau^0) = -\widetilde{G}_{IJ} \widetilde{H}_{\alpha}^{;J} \quad ,} \tag{58}$$

where $\widetilde{G}_{IJ}$ is the inverse matrix to $\widetilde{G}^{IJ} = \widetilde{H}_{0}^{;IJ}$.

10. SECOND–ORDER PERTURBATION DERIVATIVES OF TRAVEL TIME

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

$$\boxed{\tau_{,\alpha\beta}(\tau) = \tau_{,\alpha\beta}(\tau^0) + \int_{\tau^0}^{\tau} \mathrm{d}\tau \; K_{\alpha\beta} \qquad (59)}$$

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

For homogeneous Hamiltonians of the minus first degree with respect to the slowness vector, the integration kernel for the second–order perturbation derivatives of travel time can be expressed as (*Klimeš, 2002, eq. 64*)

$$K_{\alpha\beta} = -H_{,\alpha\beta} - H^{;i}_{,\alpha}\tau^{\perp}_{,i\beta} - H^{;i}_{,\beta}\tau^{\perp}_{,i\alpha} - H^{;ij}\tau^{\perp}_{,i\alpha}\tau^{\perp}_{,j\beta} \quad . \tag{60}$$

Inserting relations (25), (28) and (29), and considering biorthonormality (34), equation (60) becomes

$$K_{\alpha\beta} = -H^{;i}_{\alpha}\tau^{\perp}_{,i\beta} - H^{;i}_{\beta}\tau^{\perp}_{,i\alpha} - H^{;ij}_{0}\tau^{\perp}_{,i\alpha}\tau^{\perp}_{,j\beta} \quad . \tag{61}$$

Inserting relations (48) and (49), and considering transforms (38), (41) and (43), equation (61) can be expressed in ray–centred coordinates as

$$\boxed{K_{\alpha\beta} = -\widetilde{H}^{;I}_{\alpha}\widetilde{\tau}_{,I\beta} - \widetilde{H}^{;I}_{\beta}\widetilde{\tau}_{,I\alpha} - \widetilde{H}^{;IJ}_{0}\widetilde{\tau}_{,I\alpha}\widetilde{\tau}_{,J\beta} \quad . \qquad (62)}$$

Equation (59) cannot be integrated numerically through caustics, where $\widetilde{Q}_{IJ}$ is singular and $\widetilde{\tau}_{,I\alpha}$ in integration kernel (62) thus approach infinity. Fortunately, we may convert equation (59) analogously to *Klimeš (2002, sec. 4.2)*, but in ray–centred coordinates. Equation (59) with integration kernel (62) may be converted using dynamic ray tracing equations (45) and (46) and equation (51) with (55) into

$$\boxed{\tau_{,\alpha\beta}(\tau) = \tau_{,\alpha\beta}(\tau^0) + \left[T^{\perp}_{I\alpha}\widetilde{Q}^{-1}_{IK}\widetilde{P}^{-1}_{JK}T^{\perp}_{J\beta}\right]^{\tau}_{\tau^0} + \int_{\tau^0}^{\tau} \mathrm{d}\tau \; K^{\mathrm{caust}}_{\alpha\beta} \qquad (63)}$$

with the modified integration kernel

$$\begin{aligned} K^{\mathrm{caust}}_{\alpha\beta} =& (\widetilde{H}_{\alpha,I} + H_{\alpha}\widetilde{H}_{0,I})\,T^{\perp}_{J\beta}\widetilde{P}^{-1}_{JI} \\ &+ (\widetilde{H}_{\beta,I} + H_{\beta}\widetilde{H}_{0,I})\,T^{\perp}_{J\alpha}\widetilde{P}^{-1}_{JI} - \widetilde{\widetilde{H}}_{0,KL}T^{\perp}_{I\alpha}\widetilde{P}^{-1}_{IK}T^{\perp}_{J\beta}\widetilde{P}^{-1}_{JL} \quad . \end{aligned} \tag{64}$$

Inserting (47) into equation (64), the modified integration kernel reads

$$\boxed{\begin{aligned} K^{\mathrm{caust}}_{\alpha\beta} =& (\widetilde{H}_{\alpha,I} + H_{\alpha}\widetilde{H}_{0,I})\,T^{\perp}_{J\beta}\widetilde{P}^{-1}_{JI} \\ &+ (\widetilde{H}_{\beta,I} + H_{\beta}\widetilde{H}_{0,I})\,T^{\perp}_{J\alpha}\widetilde{P}^{-1}_{JI} - (\widetilde{H}_{0,KL} + 2\widetilde{H}_{0,I}\widetilde{H}_{0,K})T^{\perp}_{I\alpha}\widetilde{P}^{-1}_{IK}T^{\perp}_{J\beta}\widetilde{P}^{-1}_{JL} \; . \quad (65) \end{aligned}}$$

Combining equations (59) and (63) enables the optimization of calculating the second–order perturbation derivatives of travel time by numerical quadrature. The second–order perturbation derivatives of travel time are then accurately numerically calculated through caustics, although they are infinite at the caustics.

The second–order perturbation derivatives of travel time, calculated by quadratures (59) and (63), can be inserted into equation (20) for the travel–time errors due to the anisotropic–common–ray approximation, and into equation (21) for the travel–time errors due to the isotropic–common–ray approximation.

Acknowledgements: The authors are grateful to Ivan Pšenčík and two anonymous reviewers whose comments enabled the improvement and abbreviation of this paper.

The research has been supported by the Grant Agency of the Czech Republic under Contract 205/04/1104, by the Grant Agency of the Charles University under Contract 375/2004/B-GEO/MFF, and by the members of the consortium "Seismic Waves in Complex 3–D Structures" (see "http://sw3d.mff.cuni.cz").

References

Bakker P.M., 2002. Coupled anisotropic shear wave raytracing in situations where associated slowness sheets are almost tangent. *Pure Appl. Geophys.*, **159**, 1403–1417.

Baumgärtel H., 1985. *Analytic Perturbation Theory for Matrices and Operators.* Birkhäuser, Basel.

Bulant P. and Klimeš L., 2002. Numerical algorithm of the coupling ray theory in weakly anisotropic media. *Pure Appl. Geophys.*, **159**, 1419–1435.

Bulant P. and Klimeš L., 2004. Comparison of quasi–isotropic approximations of the coupling ray theory with the exact solution in the 1–D anisotropic "oblique twisted crystal" model. *Stud. Geophys. Geod.*, **48**, 97–116.

Bulant P. and Klimeš L., 2006. Numerical comparison of the isotropic–common–ray and anisotropic–common–ray approximations of the coupling ray theory. *Seismic Waves in Complex 3–D Structures, Report 16*, Dep. Geophys., Charles Univ., Prague, 155–178, online at "http://sw3d.mff.cuni.cz".

Červený V., 1972. Seismic rays and ray intensities in inhomogeneous anisotropic media. *Geophys. J. R. Astr. Soc.*, **29**, 1–13.

Červený V., 2001. *Seismic Ray Theory.* Cambridge Univ. Press, Cambridge.

Coates R.T. and Chapman C.H., 1990. Quasi–shear wave coupling in weakly anisotropic 3–D media. *Geophys. J. Int.*, **103**, 301–320.

Klimeš L., 1994. Transformations for dynamic ray tracing in anisotropic media. *Wave Motion*, **20**, 261–272.

Klimeš L., 2002. Second–order and higher–order perturbations of travel time in isotropic and anisotropic media. *Stud. Geophys. Geod.*, **46**, 213–248.

Klimeš L., 2006a. Ray–centred coordinate systems in anisotropic media. *Stud. Geophys. Geod.*, **50**, 431–447.

Klimeš L., 2006b. Common–ray tracing and dynamic ray tracing for S waves in a smooth elastic anisotropic medium. *Stud. Geophys. Geod.*, **50**, 449–461.

Klimeš L. and Bulant P., 2004. Errors due to the common ray approximations of the coupling ray theory. *Stud. Geophys. Geod.*, **48**, 117–142.

Murdock J.A., 1999. *Perturbations. Theory and Methods.* SIAM, Philadelphia.

Pšenčík I., 1998. Green's functions for inhomogeneous weakly anisotropic media. *Geophys. J. Int.*, **135**, 279–288.

Tarantola A., 1987. Inversion of travel times and seismic waveforms. In: Nolet G. (Ed.): *Sesmic Tomography*, D. Reidel Publ. Co., Dordrecht, 135–157.

Thomson C.J., Kendall J-M. and Guest W.S., 1992. Geometrical theory of shear–wave splitting: corrections to ray theory for interference in isotropic/anisotropic transitions. *Geophys. J. Int.*, **108**, 339–363.

Vavryčuk V., 2001. Ray tracing in anisotropic media with singularities. *Geophys. J. Int.*, **145**, 265–276.

Vavryčuk V., 2003. Behavior of rays near singularities in anisotropic media. *Phys. Rev. B*, **67**, 054105-1–054105-8.