# Common ray tracing and dynamic ray tracing for S waves in a smooth elastic anisotropic medium

**Luděk Klimeš**

*Department of Geophysics, Charles University, Ke Karlovu 3, 121 16 Praha 2, Czech Republic, Fax: +420-22191 1214, E-mail: klimes@sw3d.mff.cuni.cz*

## Summary

Very practical reference rays for calculating S waves by means of the coupling ray theory are anisotropic common S–wave rays. The equations required for common S–wave ray tracing in a smooth elastic anisotropic medium, and for the corresponding dynamic ray tracing, are presented in a form suitable for numerical coding. The proposed algorithm has been coded, and two–point anisotropic common S–wave travel times have been numerically calculated by anisotropic common S–wave ray tracing in a test example. The computed two–point anisotropic common S–wave travel times are compared with the second–order travel–time perturbations from isotropic rays to anisotropic common S–wave rays.

## Keywords

Travel time, ray tracing, dynamic ray tracing, geometrical spreading, coupling ray theory, seismic anisotropy, inhomogeneous media.

## 1. Introduction

The *coupling ray theory*, applicable to 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).

It has been demonstrated that the coupling ray theory along *anisotropic reference rays* yields more accurate results for S waves than the anisotropic ray theory (Bulant, Klimeš & Pšenčík 1999; Bulant & Klimeš 2002b). On the other hand, the *common ray approximation* for S waves considerably simplifies the coding of the coupling ray theory and numerical calculations. 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 linear perturbation from the common reference ray is usually applied. The common ray approximation may thus introduce errors in travel times due to the perturbation. These travel–time errors can deteriorate the coupling ray theory solution at high frequencies. The errors considerably depend on the degree of anisotropy and on the deviation of the reference ray path from the ray paths of the anisotropic ray theory.

In the commonly used *isotropic common ray approximation*, the isotropic ray theory rays are used as the reference rays for the coupling ray theory. Bakker (2002) proposed the *anisotropic common ray approximation*, in which the anisotropic common S–wave ray is traced using the averaged Hamiltonian of both S–wave polarizations.

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Klimeš & Bulant (2002) estimated the errors due to the isotropic common ray and anisotropic common ray approximations using the second–order travel–time perturbations, and demonstrated the advantages of the anisotropic common ray approximation on a numerical example.

This paper is devoted to the equations required for anisotropic P–wave ray tracing and for anisotropic common S–wave ray tracing in a smooth elastic anisotropic medium. A ray tracing algorithm is not complete without the dynamic ray tracing equations, because the dynamic ray tracing equations are required for two–point ray tracing and for the calculation of amplitudes. We thus supplement the ray tracing equations with the equations for the anisotropic P–wave dynamic ray tracing and anisotropic common S–wave dynamic ray tracing, including the equations for the corresponding Hamiltonians and their first and second derivatives. Considerable attention is paid to the dynamic ray tracing in ray–centred coordinates, and to the choice of a particular ray–centred coordinate system. All equations are expressed in a form suitable for numerical coding.

A common S–wave dynamic ray tracing algorithm based on the presented equations and suitable for the modification of the isotropic "complete ray tracing" algorithm (Červený, Klimeš & Pšenčík 1988) is proposed. The proposed algorithm has been coded, and two–point anisotropic common S–wave travel times have been numerically calculated by anisotropic common S–wave ray tracing in a test example. The calculated two–point travel times are compared with the second–order travel–time perturbations from isotropic rays to anisotropic common S–wave rays.

## 2. Partial phase–space derivatives of the eigenvalues of the Christoffel matrix

The Christoffel matrix is

$$\Gamma_{ij}(x^m,p_n) = a_{ikjl}(x^m)\,p_k p_l \quad , \tag{1}$$

where $x^m$ are the Cartesian coordinates, $a_{ijkl}(x_m)$ are the density–normalized elastic moduli, and $p_i$ are the components of the slowness vector.

We denote by $'$ or $^\star$ partial phase–space derivatives, i.e. the derivatives with respect to $x^m$ and $p_n$. Both $\Gamma'_{ij}$ and $\Gamma^\star_{ij}$ then stand for the first–order derivatives

$$\Gamma_{ij,k} \equiv \frac{\partial \Gamma_{ij}}{\partial x^k} = \frac{\partial a_{imjn}}{\partial x^k} p_m p_n \tag{2}$$

or

$$\Gamma_{ij}^{,k} \equiv \frac{\partial \Gamma_{ij}}{\partial p_k} = (a_{ikjm} + a_{imjk})p_m \quad . \tag{3}$$

Analogously, $\Gamma'^\star_{ij}$ stands for the second–order derivatives

$$\Gamma_{ij,kl} \equiv \frac{\partial^2 \Gamma_{ij}}{\partial x^k \partial x^l} = \frac{\partial^2 a_{imjn}}{\partial x^k \partial x^l} p_m p_n \tag{4}$$

or

$$\Gamma_{ij,k}^{,l} \equiv \frac{\partial^2 \Gamma_{ij}}{\partial x^k \partial p_l} = \frac{\partial (a_{iljm} + a_{imjl})}{\partial x^k} p_m \tag{5}$$

or

$$\Gamma_{ij}^{,kl} \equiv \frac{\partial^2 \Gamma_{ij}}{\partial p_k \partial p_l} = a_{ikjl} + a_{iljk} \tag{6}$$

(Červený 2001, eq. 4.14.8).

Throughout this paper, a subscript following a comma denotes the partial spatial derivative and a superscript following a comma denotes the partial derivative with respect to the slowness vector.

Three eigenvalues $G_{(a)}$ and the corresponding eigenvectors $g_{i(a)}$ of the Christoffel matrix are defined by equations

$$g_{i(a)} G_{(a)} = \Gamma_{ij} g_{j(a)} \tag{7}$$

and

$$g_{i(a)} g_{i(a)} = 1 \quad . \tag{8}$$

No implicit summation is applied to the subscripts in parentheses throughout this paper. Note that we shall use $(a)=(1)$ and $(a)=(2)$ for S waves, and $(a)=(3)$ for the P wave.

The eigenvectors are mutually perpendicular,

$$g_{i(a)} g_{i(b)} = 0 \quad \text{for} \quad b \neq a \quad . \tag{9}$$

Differentiating (7) with respect to $x^m$ or $p_n$ we arrive at

$$g'_{i(a)} G_{(a)} + g_{i(a)} G'_{(a)} = \Gamma'_{ij} g_{j(a)} + \Gamma_{ij} g'_{j(a)} \quad . \tag{10}$$

$$g'^{\star}_{i(a)} G_{(a)} + g'_{i(a)} G^{\star}_{(a)} + g^{\star}_{i(a)} G'_{(a)} + g_{i(a)} G'^{\star}_{(a)} = \Gamma'^{\star}_{ij} g_{j(a)} + \Gamma'_{ij} g^{\star}_{j(a)} + \Gamma^{\star}_{ij} g'_{j(a)} + \Gamma_{ij} g'^{\star}_{j(a)} \quad . \tag{11}$$

Differentiating (8) with respect to $x^m$ or $p_n$ we arrive at

$$g_{i(a)} g'_{i(a)} = 0 \quad . \tag{12}$$

Multiplying (7) by $g_{i(a)}$ and considering (8),

$$G_{(a)} = g_{i(a)} \Gamma_{ij} \; g_{j(a)} \quad . \tag{13}$$

Multiplying (10) by $g_{i(a)}$ and considering (7), (8), (12),

$$G'_{(a)} = g_{i(a)} \Gamma'_{ij} g_{j(a)} \quad . \tag{14}$$

Multiplying (11) by $g_{i(a)}$ and considering (7), (8), (12),

$$G'^{\star}_{(a)} = g_{i(a)} \Gamma'^{\star}_{ij} g_{j(a)} + g_{i(a)} \Gamma'_{ij} g^{\star}_{j(a)} + g_{i(a)} \Gamma^{\star}_{ij} g'_{j(a)} \quad . \tag{15}$$

Multiplying (10) by $g_{i(b)}$, $b \neq a$ and considering (7), (9),

$$g_{i(b)} g'_{i(a)} G_{(a)} = g_{i(b)} \Gamma'_{ij} g_{j(a)} + g_{i(b)} g'_{i(a)} G_{(b)} \quad . \tag{16}$$

Equations (8), (9), (12) and (16) yield (Červený 2001, eqs. 4.14.9 and 4.14.10).

$$g'_{i(a)} = \sum_{b \neq a} g_{i(b)} \frac{g_{j(b)} \Gamma'_{jk} g_{k(a)}}{G_{(a)} - G_{(b)}} \quad . \tag{17}$$

We transform the Christoffel matrix (1), its first–order derivatives (2), (3), and second–order derivatives (4), (5), (6) into the eigenvectors,

$$\Gamma_{(a\,b)} = g_{i(a)} \Gamma_{ij} g_{j(b)} \quad , \tag{18}$$

$$\Gamma'_{(a\,b)} = g_{i(a)} \Gamma'_{ij} g_{j(b)} \quad , \tag{19}$$

$$\Gamma'^{\star}_{(a\,b)} = g_{i(a)} \Gamma'^{\star}_{ij} g_{j(b)} \quad . \tag{20}$$

Equation (13) may then be expressed as

$$G_{(a)} = \Gamma_{(a\,a)} \quad , \tag{21}$$

equation (14) as

$$G'_{(a)} = \Gamma'_{(a\,a)} \quad , \tag{22}$$

and equation (15) with (17) as

$$G'^{\star}_{(a)} = \Gamma'^{\star}_{(a\,a)} + 2 \sum_{b \neq a} \frac{\Gamma'_{(a\,b)} \Gamma^{\star}_{(a\,b)}}{G_{(a)} - G_{(b)}} \quad . \tag{23}$$

Equations (2)–(6), (19), (20), (22) and (23) are suitable for the numerical calculation of the first and second partial phase–space derivatives of the eigenvalues of the Christoffel matrix.

## 3. Hamiltonian and its partial phase–space derivatives

For arithmetic averaging of the Hamiltonians of both S–wave polarizations, we consider homogeneous Hamiltonians of arbitrary degree $N$. The averaged Hamiltonian is then also homogeneous and of degree $N$. According to Euler's theorem on homogeneous functions, the parameter along rays is then proportional to the travel time. We thus choose the value of the Hamiltonian in the stationary Hamilton–Jacobi equation so that the parameter along rays is equal to the travel time,

$$H(x_m, \tau_{,n}) = \frac{1}{N} \quad , \tag{24}$$

where $N$ is the degree of the Hamiltonian $H(x_m, p_n)$, homogeneous with respect to slowness vector $p_i$.

The homogeneous Hamiltonian of degree $N$ for standard anisotropic ray tracing is

$$H_{(a)} = \tfrac{1}{N} (G_{(a)})^{\frac{N}{2}} \quad , \tag{25}$$

its first partial phase–space derivatives are

$$H'_{(a)} = \tfrac{1}{2} G'_{(a)} (G_{(a)})^{\frac{N}{2}-1} \quad , \tag{26}$$

and its second partial phase–space derivatives are

$$H'^{\star}_{(a)} = \tfrac{1}{2} G'^{\star}_{(a)} (G_{(a)})^{\frac{N}{2}-1} + \tfrac{N-2}{4} G'_{(a)} G^{\star}_{(a)} (G_{(a)})^{\frac{N}{2}-2} \quad . \tag{27}$$

For common S–wave ray tracing, we shall consider the averaged Hamiltonian of both S–wave polarizations,

$$H = \tfrac{1}{2N} [(G_{(1)})^{\frac{N}{2}} + (G_{(2)})^{\frac{N}{2}}] \quad . \tag{28}$$

Note that Bakker (2002) considered $N = 2$, whereas Klimeš & Bulant (2002) considered $N = -1$, which is better suited for travel–time perturbations. The first partial phase–space derivatives are

$$H' = \tfrac{1}{4} [G'_{(1)} (G_{(1)})^{\frac{N}{2}-1} + G'_{(2)} (G_{(2)})^{\frac{N}{2}-1}] \quad , \tag{29}$$

and the second partial phase–space derivatives are

$$H'^{\star} = \frac{1}{4} \left[ G'^{\star}_{(1)} (G_{(1)})^{\frac{N}{2}-1} + G'^{\star}_{(2)} (G_{(2)})^{\frac{N}{2}-1} \right] + \frac{N-2}{8} \left[ G'_{(1)} G^{\star}_{(1)} (G_{(1)})^{\frac{N}{2}-2} + G'_{(2)} G^{\star}_{(2)} (G_{(2)})^{\frac{N}{2}-2} \right] \quad . \tag{30}$$

We express the second derivatives of the Hamiltonian in terms of the derivatives of the Christoffel matrix using equations (22) and (23),

$$H'^{\star} = \frac{1}{4}\left[\Gamma'^{\star}_{(11)}(G_{(1)})^{\frac{N}{2}-1} + \Gamma'^{\star}_{(22)}(G_{(2)})^{\frac{N}{2}-1}\right] + \frac{\Gamma'_{(13)}\Gamma^{\star}_{(13)}(G_{(1)})^{\frac{N}{2}-1}}{2\,(G_{(1)}-G_{(3)})} + \frac{\Gamma'_{(23)}\Gamma^{\star}_{(23)}(G_{(2)})^{\frac{N}{2}-1}}{2\,(G_{(2)}-G_{(3)})}$$

$$+\Gamma'_{(12)}\Gamma^{\star}_{(12)}\frac{(G_{(1)})^{\frac{N}{2}-1}-(G_{(2)})^{\frac{N}{2}-1}}{2\,(G_{(1)}-G_{(2)})} + \frac{N-2}{8}\left[\Gamma'_{(11)}\Gamma^{\star}_{(11)}(G_{(1)})^{\frac{N}{2}-2} + \Gamma'_{(22)}\Gamma^{\star}_{(22)}(G_{(2)})^{\frac{N}{2}-2}\right] \quad . \tag{31}$$

The term with $G_{(1)} - G_{(2)}$ in the denominator is possibly singular. It is thus desirable to carry out the division by $G_{(1)} - G_{(2)}$ analytically. For $N=2$,

$$\frac{(G_{(1)})^{\frac{N}{2}-1}-(G_{(2)})^{\frac{N}{2}-1}}{G_{(1)}-G_{(2)}} = 0 \quad . \tag{32}$$

For $N=1$,

$$\frac{(G_{(1)})^{\frac{N}{2}-1}-(G_{(2)})^{\frac{N}{2}-1}}{G_{(1)}-G_{(2)}} = -\frac{1}{(G_{(1)})^{\frac{1}{2}}[(G_{(1)})^{\frac{1}{2}}+(G_{(2)})^{\frac{1}{2}}](G_{(2)})^{\frac{1}{2}}} \quad . \tag{33}$$

For $N=-1$,

$$\frac{(G_{(1)})^{\frac{N}{2}-1}-(G_{(2)})^{\frac{N}{2}-1}}{G_{(1)}-G_{(2)}} = -\frac{G_{(1)}+(G_{(1)}G_{(2)})^{\frac{1}{2}}+G_{(2)}}{(G_{(1)})^{\frac{3}{2}}[(G_{(1)})^{\frac{1}{2}}+(G_{(2)})^{\frac{1}{2}}](G_{(2)})^{\frac{3}{2}}} \quad . \tag{34}$$

For $N=-2$,

$$\frac{(G_{(1)})^{\frac{N}{2}-1}-(G_{(2)})^{\frac{N}{2}-1}}{G_{(1)}-G_{(2)}} = -\frac{G_{(1)}+G_{(2)}}{(G_{(1)})^{2}(G_{(2)})^{2}} \quad . \tag{35}$$

Dynamic ray tracing is often performed in ray centred coordinates. The transformation of the second phase–space derivatives of the Hamiltonian from Cartesian to ray centred coordinates depends on the degree $N$ of the homogeneous Hamiltonian (Klimeš 2002a). To simplify the transformation, it may be useful to convert homogeneous Hamiltonian $H(x_m,p_n)$ of arbitrary degree $N$ into homogeneous Hamiltonian $\widetilde{H}(x_m,p_n)$ of a fixed degree. Here we choose the second degree for $\widetilde{H}(x_m,p_n)$, similarly as Klimeš (1994). The homogeneous Hamiltonian of the second degree is

$$\widetilde{H} = \tfrac{1}{2}\,(NH)^{\frac{2}{N}} \quad , \tag{36}$$

its first partial phase–space derivatives are

$$\widetilde{H}' = H'\,(NH)^{\frac{2}{N}-1} \quad , \tag{37}$$

and its second partial phase–space derivatives are

$$\widetilde{H}'^{\star} = H'^{\star}\,(NH)^{\frac{2}{N}-1} + (2-N)\,H'H^{\star}\,(NH)^{\frac{2}{N}-2} \quad . \tag{38}$$

For a P wave, we may directly put $\widetilde{H} = G_{(3)}$, $\widetilde{H}' = G'_{(3)}$ and $\widetilde{H}'^{\star} = G'^{\star}_{(3)}$.

## 4. Ray tracing system and dynamic ray tracing system in Cartesian coordinates

The ray tracing equations may be expressed in the form of Hamilton's equations

$$\dot{x}^k = H^{,k} \quad , \tag{39}$$

$$\dot{p}_k = -H_{,k} \quad , \tag{40}$$

where a subscript following a comma denotes the partial spatial derivative and a superscript following a comma denotes the partial derivative with respect to the slowness vector,

$$H_{,i} \equiv \frac{\partial H}{\partial x^i} \quad , \qquad H^{,i} \equiv \frac{\partial H}{\partial p_i} \quad . \tag{41}$$

This notation of the partial phase space derivatives has already been introduced in Section 2, and will be used throughout this paper.

The dot stands for the derivative $\partial/\partial\gamma_3$ along the ray. Since we have chosen a homogeneous Hamiltonian and have chosen its constant value to be given by (24), we have

$$\dot{\tau} = H^{,k} p_k = 1 \quad . \tag{42}$$

The dot then represents the derivative $\partial/\partial\tau$ with respect to the travel time.

The dynamic ray tracing system in Cartesian coordinates (Červený 1972) can be obtained by differentiating ray tracing equations (39) and (40) with respect to ray parameter $\gamma$,

$$\dot{Q}^i = H^{,i}_{,j} Q^j + H^{,ij} P_j \quad , \tag{43}$$

$$\dot{P}_i = -H_{,ij} Q^j - H^{,j}_{,i} P_j \quad , \tag{44}$$

where

$$Q^i = \frac{\partial x^i}{\partial \gamma} \quad , \tag{45}$$

$$P_i = \frac{\partial p_i}{\partial \gamma} \quad . \tag{46}$$

## 5. Dynamic ray tracing system in ray–centred coordinates

Ray–centred coordinates were applied to the polarization of electromagnetic waves by Luneburg (1944) and to dynamic ray tracing in isotropic media by Babich & Buldyrev (1972) and Popov & Pšenčík (1978a; 1978b), and then to dynamic ray tracing in anisotropic media by Hanyga (1982), Kendall, Guest & Thomson (1992) and Klimeš (1994).

The $q^3$–coordinate line of ray–centred coordinates $q^m$ is the axial ray parametrized by parameter

$$q^3 = q_0^3 + \int_{\tau_0}^{\tau} w \, \mathrm{d}\tau \quad . \tag{47}$$

For example, the parameter may be travel time $q^3 = \tau$ if $w = 1$, or arclength $q^3 = s$ if $w$ is the ray velocity, $w = \sqrt{H^{,i} H^{,i}}$ . The $q^A$ coordinates lie, for fixed $q^3$, in the wavefront tangent plane. The Cartesian coordinates corresponding to $q^m$ are

$$x^i = x_0^i(q^3) + h_M^i(q^3)\, q^M \quad , \tag{48}$$

where $x_0^i(\tau)$ are points of the axial ray. This is both the definition of the ray–centred coordinates, and the transformation equation from the ray–centred to Cartesian coordinates. The transformation matrices, taken at the central ray, are

$$t_m^i = \frac{\partial x^i}{\partial q^m} \quad , \qquad \hat{t}_i^m = \frac{\partial q^m}{\partial x^i} \quad . \tag{49}$$

Transformation matrices (49) are related by equations

$$t_M^i = h_M^i \quad , \qquad t_3^i = w^{-1} h_3^i \quad , \qquad \hat{t}_i^M = \hat{h}_i^M \quad , \qquad \hat{t}_i^3 = w \hat{h}_i^3 \tag{50}$$

to analogous transformation matrices $h_m^i$ and $\hat{h}_i^m$, formally introduced for $w = 1$. In this paper, the dynamic ray tracing in ray–centred coordinates is restricted to coordinates $q_1$ and $q_2$ only. The choice of $q_3$ then does not influence the dynamic ray tracing. We shall thus substitute $h_m^i$ and $\hat{h}_i^m$ for $t_m^i$ and $\hat{t}_i^m$ in the rest of this paper.

The "contravariant basis vectors" $h_1^i$, $h_2^i$, $h_3^i$ and the "covariant basis vectors" $\hat{h}_i^1$, $\hat{h}_i^2$, $\hat{h}_i^3$ of the ray–centred coordinate system are defined by equations (Klimeš 1994, eq. 23)

$$h_3^i = H^{,i} \quad , \tag{51}$$

$$\hat{h}_i^3 = p_i \quad , \tag{52}$$

$$h_a^i \hat{h}_i^b = \delta_a^b \quad . \tag{53}$$

The first two contravariant basis vectors $h_1^i$, $h_2^i$ of the ray–centred coordinate system are tangent to the wavefront, the third contravariant basis vector $h_3^i$ is tangent to the ray. The first two covariant basis vectors $\hat{h}_i^1$, $\hat{h}_i^2$ of the ray–centred coordinate system are perpendicular to the ray, the third covariant basis vector $\hat{h}_i^3$ is perpendicular to the wavefront. Whereas basis vectors $h_3^i$ and $\hat{h}_i^3$ are uniquely determined by equations (51) and (52), we may either choose the contravariant basis vectors $h_1^i$ and $h_2^i$ arbitrarily in the wavefront tangent plane, or choose the covariant basis vectors $\hat{h}_i^1$ and $\hat{h}_i^2$ arbitrarily in the plane perpendicular to the ray velocity vector $h_3^i$.

If the contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_1$ are known, the covariant basis vectors $\hat{\mathbf{h}}^1$ and $\hat{\mathbf{h}}^2$ are given by relations

$$\hat{\mathbf{h}}^1 = \frac{\mathbf{h}_3 \times \mathbf{h}_2}{\mathbf{h}_1^{\mathrm{T}} (\mathbf{h}_3 \times \mathbf{h}_2)} \quad , \tag{54}$$

$$\hat{\mathbf{h}}^2 = \frac{\mathbf{h}_3 \times \mathbf{h}_1}{\mathbf{h}_2^{\mathrm{T}} (\mathbf{h}_3 \times \mathbf{h}_1)} \quad . \tag{55}$$

If the covariant basis vectors $\hat{\mathbf{h}}^1$ and $\hat{\mathbf{h}}^2$ are known, the contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_1$ are given by relations

$$\mathbf{h}_1 = \frac{\mathbf{p} \times \hat{\mathbf{h}}^2}{\hat{\mathbf{h}}_1^{\mathrm{T}} (\mathbf{p} \times \hat{\mathbf{h}}^2)} \quad , \tag{56}$$

$$\mathbf{h}_2 = \frac{\mathbf{p} \times \hat{\mathbf{h}}^1}{\hat{\mathbf{h}}_2^{\mathrm{T}} (\mathbf{p} \times \hat{\mathbf{h}}^1)} \quad . \tag{57}$$

The $4 \times 4$ dynamic ray tracing system in ray–centred coordinates reads (Klimeš 1994, eq. 60)

$$\dot{Q}^M_{(q)} = H^{(q),M}_{,N} Q^N_{(q)} + H^{,MN}_{(q)} P^{(q)}_N \quad , \tag{58}$$

$$\dot{P}^{(q)}_M = -H^{(q)}_{,MN} Q^N_{(q)} - H^{(q),N}_{,M} P^{(q)}_N \quad , \tag{59}$$

where

$$Q^M_{(q)} = \frac{\partial q^M}{\partial \gamma} \quad , \tag{60}$$

$$P^{(q)}_M = \frac{\partial}{\partial \gamma} \left( \frac{\partial \tau}{\partial q_M} \right) \quad . \tag{61}$$

The second phase–space derivatives of the Hamiltonian in ray–centred coordinates are given by relations (Klimeš 1994, eqs. 51a, 51b, 51c; Červený 2001, eq. 4.2.78)

$$H^{(q)}_{,MN} = h^j_M [H_{,jk} - (N-1) H_{,j} H_{,k}] h^k_N \quad , \tag{62}$$

$$H^{(q),N}_{,M} = h^j_M H^{,k}_{,j} \hat{h}^N_k - d^N_M \quad , \tag{63}$$

$$H^{,MN} = \hat{h}^M_j H^{,jk} \hat{h}^N_k \quad . \tag{64}$$

Nine coefficients

$$d^a_b = \hat{h}^a_i \dot{h}^i_b = -h^i_b \dot{\hat{h}}^a_i \tag{65}$$

describe the evolution of the ray–centred coordinates along the ray,

$$\dot{h}^i_b = \dot{h}^i_a d^a_b \quad , \tag{66}$$

$$\dot{\hat{h}}^a_i = -\dot{\hat{h}}^b_i d^a_b \quad . \tag{67}$$

The four coefficients $d^N_M$ in equation (63) thus depend on the choice of basis vectors $h^i_1$, $h^i_2$ (or $\hat{h}^1_i$, $\hat{h}^2_i$) along the ray, which will be discussed in the next section.

On the other hand, the choice of the four coefficients $d^N_M$ uniquely determine the evolution of the basis vectors of the ray–centred coordinate system along the ray if the basis vectors are given at the initial point of the ray, because the remaining five coefficients $d^N_3$, $d^3_M$, $d^3_3$ are determined by definition (51) and (52). Evolution equations

$$\dot{h}^i_3 = H^{,i}_{,j} H^{,j} - H^{,ij} H_{,j} \quad , \tag{68}$$

$$\dot{\hat{h}}^3_i = -H_{,i} \quad , \tag{69}$$

follow from definition (51) and (52) and ray tracing system (39) and (40). Coefficients $d_3^a$ and $d_b^3$ are thus uniquely determined,

$$d_3^a = \hat{h}_i^a (H_{,j}^{,i} H^{,j} - H^{,ij} H_{,j}) \quad , \tag{70}$$

$$d_b^3 = H_{,i} h_b^i \quad , \tag{71}$$

$$d_3^3 = H_{,i} H^{,i} \quad . \tag{72}$$

## 6. Basis vectors of the ray–centred coordinate system

There are many possibilities how to choose the basis vectors $h_1^i$, $h_2^i$ (or $\hat{h}_i^1$, $\hat{h}_i^2$) along the ray in an anisotropic medium (Hanyga 1982; Kendall, Guest & Thomson 1992; Klimeš 1994). Many particular choices have their own advantages for particular applications. Sections 6.1 and 6.2 include some notes related to the basis vectors. In Sections 6.3 to 6.8, we briefly list five particular choices of the basis vectors. The choice preferred in Section 7 for the modification of the isotropic "complete ray tracing" algorithm (Červený, Klimeš & Pšenčík 1988) is described in Section 6.6. Other parts of Section 6 are of little importance for our numerical implementation of the algorithm, but may be interesting for other applications.

### 6.1. Notes on the "orthonormality" of the basis vectors

Four "free" coefficients $d_B^A$ characterize a particular choice of the ray–centred coordinate system. Three coefficients $d_1^1$, $d_2^2$ and $\frac{1}{2}(d_2^1 + d_1^2)$, forming the symmetric part of the $2\times2$ matrix $d_B^A$, are determined by the "orthonormality relations" between $h_1^i$ and $h_2^i$. One coefficient $\frac{1}{2}(d_2^1 - d_1^2)$, forming the skew part of the $2\times2$ matrix $d_B^A$, characterizes the torsion of the ray–centred coordinate system. Under the orthonormality relations we understand relations

$$h_A^i g_{ij} h_B^j = \delta_{AB} \quad , \tag{73}$$

or

$$\hat{h}_i^A g^{ij} \hat{h}_j^B = \delta^{AB} \quad , \tag{74}$$

where $g_{ij}$ or $g^{ij}$ is some metric tensor. Differentiation of (73) and (74) yields

$$\dot{h}_A^i g_{ij} h_B^j + h_A^i g_{ij} \dot{h}_B^j = -h_A^i \dot{g}_{ij} h_B^j \quad , \tag{75}$$

and

$$\dot{\hat{h}}_i^A g^{ij} \hat{h}_j^B + \hat{h}_i^A g^{ij} \dot{\hat{h}}_j^B = -\hat{h}_i^A \dot{g}^{ij} \hat{h}_j^B \quad . \tag{76}$$

Then

$$d_B^A + d_A^B = -d_A^3 h_3^i g_{ij} h_B^j - d_B^3 h_3^i g_{ij} h_A^j - h_A^i \dot{g}_{ij} h_B^j \quad , \tag{77}$$

and

$$d_B^A + d_A^B = -d_3^A \hat{h}_i^3 g^{ij} \hat{h}_j^B - d_3^B \hat{h}_i^3 g^{ij} \hat{h}_j^B + \hat{h}_i^A \dot{g}^{ij} \hat{h}_j^B \quad . \tag{78}$$

## 6.2. Notes on the evolution equations for the basis vectors

The evolution differential equations for the basis vectors are often expressed in the form

$$\dot{h}^i_A = D^i_j h^j_A \tag{79}$$

for contravariant basis vectors $h^j_1$, $h^j_2$, or in the form

$$\dot{\hat{h}}^A_i = \hat{D}^j_i \hat{h}^A_j \tag{80}$$

for covariant basis vectors $\hat{h}^1_j$, $\hat{h}^2_j$. Since we do not expect to use equations (79) or (80) here for basis vectors $h^j_3$ or $\hat{h}^3_j$, respectively, coefficients $D^i_j$ and $\hat{D}^j_i$ are not uniquely determined by the basis vectors. Equations (79) or (80) are invariant with respect to gauge transformations

$$D^i_j \longrightarrow D^i_j + \xi^i p_j \quad , \qquad \hat{D}^j_i \longrightarrow \hat{D}^j_i + \hat{\xi}_i H^{,j} \quad , \tag{81}$$

where $\xi^i$ and $\hat{\xi}_i$ are arbitrary vectors given along the ray.

Assume now that we have equation (79) for $h^i_A$ and wish to write equation (80) for $\hat{h}^A_i$, or vice versa. The differentiation of equation (53) along the ray yields

$$\dot{h}^i_a \hat{h}^b_i + h^i_a \dot{\hat{h}}^b_i = 0 \quad , \tag{82}$$

and consequently

$$\dot{h}^i_a = -h^i_b \dot{\hat{h}}^b_j h^j_a \quad . \tag{83}$$

Inserting (80) for $\dot{\hat{h}}^B_j$,

$$\dot{h}^i_a = -h^i_B \hat{D}^k_j \hat{h}^B_k h^j_a - h^i_3 \dot{\hat{h}}^3_j h^j_a \quad . \tag{84}$$

Considering (51)–(53) and (69),

$$\dot{h}^i_a = -(\delta^i_k - H^{,i} p_k) \hat{D}^k_j h^j_a + H^{,i} H_{,j} h^j_a \quad . \tag{85}$$

The coefficients $D^i_j$ derived from $\hat{D}^i_j$ are then

$$D^i_j = -\hat{D}^i_j + H^{,i}(\hat{D}^k_j p_k + H_{,j}) + \xi^i p_j \quad , \tag{86}$$

where $\xi^i$ is an arbitrary vector given along the ray. Analogously,

$$\dot{\hat{h}}^a_i = -\hat{h}^b_i \dot{h}^j_b \hat{h}^a_j \quad . \tag{87}$$

Inserting (79) for $\dot{h}^j_B$,

$$\dot{\hat{h}}^a_i = -\hat{h}^B_i D^j_k h^k_B \hat{h}^a_j - \hat{h}^3_i \dot{h}^j_3 \hat{h}^a_j \quad . \tag{88}$$

Considering (52)–(54),

$$\dot{\hat{h}}^a_i = -(\delta^k_i - p_i H^{,k}) D^j_k \hat{h}^a_j - p_i \dot{h}^j_3 \hat{h}^a_j \quad . \tag{89}$$

The coefficients $\hat{D}^j_i$ derived from $D^j_i$ are then

$$\hat{D}^j_i = -D^j_i + p_i(D^j_k H^{,k} - \dot{h}^j_3) + \hat{\xi}_i H^{,j} \quad , \tag{90}$$

or, inserting (68),

$$\hat{D}^j_i = -D^j_i + p_i[(D^j_k H^{,k} - H^{,j}_{,k}) H^{,k} + H^{,ij} H_{,j}] + \hat{\xi}_i H^{,j} \quad , \tag{91}$$

where $\hat{\xi}_i$ is an arbitrary vector given along the ray.

The relations between coefficients $d^A_B$, $D^i_j$ and $\hat{D}^j_i$ follow from definitions (65), (79) and (80),

$$d^A_B = \hat{h}^A_i D^i_j h^j_B = -h^i_B \hat{D}^j_i \hat{h}^A_j \quad , \tag{92}$$

$$D^i_j = h^i_a d^a_B \hat{h}^B_j + \xi^i p_j \quad , \tag{93}$$

$$\hat{D}^j_i = -\hat{h}^b_i d^A_b h^j_A + \hat{\xi}_i H^{,j} \quad , \tag{94}$$

where $\xi^i$ and $\hat{\xi}_i$ are arbitrary vectors given along the ray.

### 6.3. Wavefront–tangent and ray–normal projections of constant vectors

Hanyga (1982) introduced projection operator

$$P^i_j = \delta^i_j - h^i_3 p_j \tag{95}$$

with respect to the wave–propagation metric, projecting contravariant vectors onto the wavefront tangent plane and covariant vectors onto the plane normal to the ray. Contravariant basis vectors of the ray–centred coordinate system may then be chosen as the projections of two constant vectors $e^i_1$ and $e^i_2$ onto the wavefront tangent plane,

$$h^i_A = P^i_j e^j_A \quad . \tag{96}$$

Note that Hanyga (1982) suggested choosing $e^i_1$ and $e^i_2$ as the unit vectors in the direction of two axes selected of the three Cartesian coordinate axes. The corresponding covariant basis vectors $\hat{\mathbf{h}}^1$ and $\hat{\mathbf{h}}^2$ may be calculated using relations (54) and (55). Differentiating equation (96) with projection operator (95) along the ray, and considering definition (65) of $d^a_b$ and relation (53), we obtain equation

$$d^A_B = -\hat{h}^A_i \dot{h}^i_3 p_j e^j_B \quad . \tag{97}$$

Similarly, we may select two constant vectors $\hat{e}^1_i$ and $\hat{e}^2_i$ and project them onto the plane perpendicular to the ray,

$$\hat{h}^A_i = P^j_i \hat{e}^A_j \quad . \tag{98}$$

The corresponding contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ may be calculated using relations (56) and (57). Differentiating equation (98) with projection operator (95) along the ray, and considering definition (65) of $d^a_b$ and relation (53), we obtain equation

$$d^A_B = h^i_B \dot{p}_i h^j_3 \hat{e}^A_j \quad . \tag{99}$$

The advantage of this option is the possibility of calculating the basis vectors of the ray–centred coordinate system locally, without solving an ordinary differential equation along the ray. Unfortunately, for each couple of constant vectors $e^i_1$ and $e^i_2$ ($\hat{e}^1_i$ and $\hat{e}^2_i$), we have to switch to another couple of constant vectors if the slowness vector (ray–velocity vector) is not sufficiently deviated from the plane given by vectors $e^i_1$ and $e^i_2$ ($\hat{e}^1_i$ and $\hat{e}^2_i$). The experience with similar switching of the constant reference vectors for the determination of the basis vectors of the ray–centred coordinate system in isotropic media definitely lead Červený, Klimeš & Pšenčík (1988) to abandon this option and prefer the numerical calculation of the basis vectors by numerical integration along the ray. When approaching isotropy, this ray–centred coordinate system does not converge to the ray–centred coordinate system for isotropic media.

### 6.4. Basis vectors orthonormal with respect to the wave–propagation metric

The Finslerian contravariant wave–propagation metric tensor is given by the second derivatives of the homogeneous Hamiltonian of the second degree with respect to the slowness vector,

$$G^{ij} = \widetilde{H}^{,ij} = \tfrac{1}{2}[(NH)^{\frac{2}{N}}]^{,ij} = (NH)^{\frac{2-N}{N}}[H^{,ij} + \tfrac{2-N}{NH}H^{,i}H^{,j}] \quad . \tag{100}$$

Since $H = 1/N$ along the rays,

$$G^{ij} = [H^{,ij} + (2-N)H^{,i}H^{,j}] \tag{101}$$

along the Hamiltonian hypersurface in phase space. If relation

$$h^i_a = G^{ij}\hat{h}^a_j \quad , \tag{102}$$

which always holds for $a = 3$, also applies to $a = 1, 2$, the orthonormality relation

$$\hat{h}^a_i G^{ij}\hat{h}^b_j = \delta^{ab} \quad , \tag{103}$$

following from (53) and (103), applies to all $a$, $b$, not only to $a = 3$ or $b = 3$. Then also

$$\hat{h}^a_i = G_{ij}h^j_b \tag{104}$$

and

$$h^i_a G_{ij} h^j_b = \delta_{ab} \quad , \tag{105}$$

where the covariant metric tensor $G_{ij}$ is the matrix inverse to the contravariant metric tensor $G^{ij}$,

$$G_{ij}G^{jk} = \delta^k_i \quad . \tag{106}$$

Differentiating equation (102) along the ray and considering definition (65) of $d^a_b$, we obtain equation

$$d^a_b + d^b_a = \hat{h}^a_i \dot{G}^{ij}\hat{h}^b_j \quad , \tag{107}$$

where

$$\dot{G}^{ij} = G^{ij}_{,k}H^{,k} - G^{ij,k}H_{,k} \quad . \tag{108}$$

For $a, b = 1, 2$, equation (107) is a special case of equation (78) with $g^{ij} = G^{ij}$ and orthonormality relations (103). Coefficient $\frac{1}{2}(d^1_2 - d^2_1)$ may be obtained from additional conditions, e.g., from the additional postulates of Cartan imposed on the *parallel displacement* along a ray (Rund 1959, sec. 3.1., conditions III). Refer to Section 6.5 for a brief summary of the parallel displacement.

Note that tensor

$$G^{ij,k} = \widetilde{H}^{,ijk} = \tfrac{1}{2}[(NH)^{\frac{2}{N}}]^{,ijk} \tag{109}$$

in equation (108) is symmetric with respect to all three superscripts, and defines the contravariant *Cartan torsion tensor*

$$C^{ijk} = -\tfrac{1}{2}G^{ij,k} \tag{110}$$

(Rund 1959, eq. 3.1.11).

Relation for $G^{ij,k}$ in terms of the derivatives of a general homogeneous Hamiltonian may be obtained by differentiating equation (100) with respect to $p_k$,

$$G^{ij,k} = (NH)^{\frac{2-N}{N}}\left[H^{,ijk} + \tfrac{2-N}{NH}\left(H^{,i}H^{,jk} + H^{,j}H^{,ik} + H^{,k}H^{,ij} + \tfrac{2-2N}{NH}H^{,i}H^{,j}H^{,k}\right)\right] \quad . \tag{111}$$

Since $H = 1/N$ along the rays,

$$G^{ij,k} = \{H^{,ijk} + (2-N)[H^{,i}H^{,jk} + H^{,j}H^{,ik} + H^{,k}H^{,ij} + (2-2N)H^{,i}H^{,j}H^{,k}]\} \ . \quad (112)$$

The analogous relation for $G^{ij}_{,k}$ may be obtained by differentiating equation (100) with respect to $x^k$,

$$G^{ij}_{,k} = (NH)^{\frac{2-N}{N}}[H^{,ij}_{,k} + \tfrac{2-N}{NH}(H^{,ij}H_{,k} + H^{,i}_{,k}H^{,j} + H^{,i}H^{,j}_{,k} + \tfrac{2-2N}{NH}H^{,i}H^{,j}H_{,k})] \ . \quad (113)$$

Since $H = 1/N$ along the rays,

$$G^{ij}_{,k} = \{H^{,ij}_{,k} + (2-N)[H^{,ij}H_{,k} + H^{,i}_{,k}H^{,j} + H^{,i}H^{,j}_{,k} + (2-2N)H^{,i}H^{,j}H_{,k}]\} \ . \quad (114)$$

Inserting (108) with (112) and (114) into (107), for the symmetric part of the $2\times 2$ matrix $d^A_B$ we obtain equation

$$\tfrac{1}{2}(d^A_B + d^B_A) = \tfrac{1}{2}\hat{h}^A_i(H^{,ij}_{,k}H^{,k} - H^{,ijk}H_{,k})\hat{h}^B_j \quad , \quad (115)$$

valid for a homogeneous Hamiltonian of an arbitrary degree.

The greatest disadvantage of this option is the necessity to calculate the third partial phase–space derivatives of the Hamiltonian. When approaching isotropy, this ray–centred coordinate system does not converge to the ray–centred coordinate system for isotropic media.

### 6.5. Finslerian parallel displacement along a ray

We shall consider only the parallel displacement along a ray, not along a general curve. We shall adopt the relevant equations of Rund (1959) without deriving them.

The parallel displacement of the contravariant basis vectors along the ray can be expressed in the form

$$\dot{h}^j_a = -C^{mjn}G_{mi}G_{nk}h^i_a\dot{h}^k_3 - P^j_{ik}h^i_a\dot{x}^k \quad (116)$$

(Rund 1959, eq. 3.1.3). The analogous equation for the covariant basis vectors is

$$\dot{\hat{h}}^a_i = G_{im}C^{mjn}G_{nk}\hat{h}^a_j\dot{h}^k_3 + P^j_{ik}\hat{h}^a_j\dot{x}^k \quad . \quad (117)$$

Inserting (68), equations (116) and (117) read

$$\dot{h}^j_a = -C^{mjk}G_{mi}h^i_a\dot{p}_k - (P^j_{ik} + C^{mjn}G_{mi}G_{nr}H^{,r}_{,k})h^i_a\dot{x}^k \quad , \quad (118)$$

$$\dot{\hat{h}}^a_i = G_{im}C^{mjk}\hat{h}^a_j\dot{p}_k + (P^j_{ik} + G_{im}C^{mjn}G_{nr}H^{,r}_{,k})\hat{h}^a_j\dot{x}^k \quad . \quad (119)$$

A relatively complex expression for $P^j_{ik}$ is given by Rund (1959, eq 3.1.30), but the expression for $P^j_{ik}\dot{x}^k$ can be considerably simplified when using identity

$$C^{ijk}p_k = 0 \quad (120)$$

(Rund 1959, eq. 3.1.12), following from the zero–degree homogeneity of the metric tensor with respect to the slowness vector. Rund's (1959) equation 3.1.30 then yields

$$P^j_{ik}\dot{x}^k = \gamma^j_{ik}\dot{x}^k \quad , \quad (121)$$

where $\gamma^j_{ik}$ are defined for fixed $\dot{x}^m$ analogously as the Christoffel symbols in Riemannian geometry (Rund 1959, eq. 2.2.3). Since we calculate spatial derivatives for fixed $p_m$, we express $\gamma^j_{ik}$ in form

$$\gamma^j_{ik} = \Gamma^j_{ik} - G_{im}C^{mjr}G_{rs}\widetilde{H}^{,s}_{,k} - G_{km}C^{mjr}G_{rs}\widetilde{H}^{,s}_{,i} + G_{im}G_{kn}C^{mnr}G_{rs}\widetilde{H}^{,s}_{,j} \quad , \quad (122)$$

where $\Gamma^j_{ik}$ are defined for fixed $p_m$ analogously to the Christoffel symbols in Riemannian geometry,

$$\Gamma^j_{ik} = -\tfrac{1}{2}\left(G^{jr}_{,i}G_{rk} + G^{jr}_{,k}G_{ri} - G^{jl}G^{rs}_{,l}G_{ri}G_{sk}\right) \quad . \tag{123}$$

Considering (120), we may write

$$P^j_{ik}\dot{x}^k = \Gamma^j_{ik}\dot{x}^k - G_{im}C^{mjr}G_{rs}\widetilde{H}^{,s}_{,k}\dot{x}^k \quad . \tag{124}$$

On converting the derivatives $\widetilde{H}^{,i}_{,j}$ of the homogeneous Hamiltonian of the second degree to the derivatives of the homogeneous Hamiltonian of an arbitrary degree using equation (124), we arrive at

$$h^i_A(P^j_{ik} + G_{im}C^{mjn}G_{nr}H^{,r}_{,k}\dot{x}^k)h^j_B = h^i_A\Gamma^j_{ik}\dot{x}^k h^j_B \quad . \tag{125}$$

Equation (123) multiplied by $\dot{x}^k = G^{kr}p_r$ reads

$$\Gamma^i_{mn}\dot{x}^m = -\tfrac{1}{2}\left(G^{ik}_{,m}G_{kn}G^{mr} + G^{ir}_{,n} - G^{rk}_{,l}G_{kn}G^{il}\right)p_r \quad . \tag{126}$$

Considering the homogeneity of the Hamiltonian of the second degree used to define metric tensor $G^{ij}$,

$$\Gamma^i_{mn}\dot{x}^m = -\tfrac{1}{2}\left(G^{ik}_{,m}G_{kn}h^m_3 + \widetilde{H}^{i}_{,n} - \widetilde{H}^{k}_{,l}G_{kn}G^{il}\right) \quad . \tag{127}$$

Inserting (110), (118), (125) and (127) into (65), we obtain

$$d^A_B = \tfrac{1}{2}\hat{h}^A_i\hat{h}^B_j G^{ij,k}\dot{p}_k + \tfrac{1}{2}[G^{ij}_{,m}\hat{h}^A_i\hat{h}^B_j h^m_3 + \widetilde{H}^{i}_{,k}(\hat{h}^A_i h^k_B - \hat{h}^B_i h^k_A)] \quad . \tag{128}$$

Converting the derivatives of the homogeneous Hamiltonian of the second degree to the derivatives of the homogeneous Hamiltonian of an arbitrary degree using expressions (38), (112) and (116), and expressing $h^i_3$ and $\dot{p}_i$ in terms of the Hamiltonian, we arrive at

$$\begin{aligned} d^A_B = &-\tfrac{1}{2}[\hat{h}^A_i\hat{h}^B_j H^{,ijk} + (2-N)\delta^A_B H^{,k}]H_{,k} \\ &+\tfrac{1}{2}[H^{,ij}_{,k}\hat{h}^A_i\hat{h}^B_j H^{,k} + (2-N)\delta^A_B H_{,k}H^{,k} + H^{i}_{,k}(\hat{h}^A_i h^k_B - \hat{h}^B_i h^k_A)] \quad . \end{aligned} \tag{129}$$

Finally,

$$d^A_B = \tfrac{1}{2}\hat{h}^A_i\hat{h}^B_j(H^{,ij}_{,k}H^{,k} - H^{,ijk}H_{,k}) + \tfrac{1}{2}H^{i}_{,k}(\hat{h}^A_i h^k_B - \hat{h}^B_i h^k_A) \quad . \tag{130}$$

The symmetric part of the $2\times2$ matrix $d^A_B$ is already known from equation (115), but the skew part could not be derived without the parallel displacement. Note that the skew part of matrix (130) makes the $2\times2$ matrix of the mixed second derivatives (63) of the Hamiltonian in ray–centred coordinates symmetric.

### 6.6. Contravariant basis vectors $\mathbf{h}_1$, $\mathbf{h}_2$ orthonormal with respect to the Cartesian metric

Another option is to choose the contravariant basis vectors $h_1^i$ and $h_2^i$, which are perpendicular to the slowness vector, mutually orthonormal with respect to the Cartesian metric,

$$h_A^i h_B^i = \delta_{AB} \tag{131}$$

(Klimeš 2002b, eq. 50). The simplest way of keeping condition (131) satisfied along the ray is to choose the derivatives of both vectors in the direction of the slowness vector (Červený 2001, eq. 4.2.23),

$$\dot{h}_A^i = -\frac{p_i}{p_r p_r} \dot{p}_j h_A^j \quad . \tag{132}$$

In terms of the Hamiltonian,

$$\dot{h}_A^i = \frac{p_i}{p_r p_r} H_{,j} h_A^j \quad . \tag{133}$$

It is sufficient to calculate contravariant basis vector $\mathbf{h}_1$ by solving equation (133) numerically. Vector $\mathbf{h}_2$ is then given by relation

$$\mathbf{h}_2 = \frac{\mathbf{p} \times \mathbf{h}_1}{|\mathbf{p} \times \mathbf{h}_1|} \quad , \tag{134}$$

and vectors $\hat{\mathbf{h}}^1$ and $\hat{\mathbf{h}}^2$ by relations (54) and (55).

The equation for the covariant basis vectors may be obtained from (133) using relation (91),

$$\dot{\hat{h}}_i^a = -(H_{,i} - p_i H^{,k} H_{,k}) \frac{p_j}{p_r p_r} \hat{h}_j^a - p_i (H^{,j}_{,k} H^{,k} - H^{,jk} H_{,k}) \hat{h}_j^a \quad . \tag{135}$$

The $2\times2$ submatrix of the $3\times3$ matrix (65) is

$$d_B^A = \frac{p_i \hat{h}_i^A}{p_r p_r} H_{,j} h_B^j \quad . \tag{136}$$

This is a very comfortable option for coding, because equation (133) contains only the first derivatives of the Hamiltonian. When approaching isotropy, this ray–centred coordinate system with $w = \sqrt{H^{,i} H^{,i}}$ in (47) converges to the ray–centred coordinate system for isotropic media.

### 6.7. Covariant basis vectors $\hat{\mathbf{h}}^1$, $\hat{\mathbf{h}}^2$ orthonormal with respect to the Cartesian metric

Another option is to choose the covariant basis vectors $\hat{h}_i^1$ and $\hat{h}_i^2$, which are perpendicular to the ray, mutually orthonormal with respect to the Cartesian metric,

$$\hat{h}_i^A \hat{h}_i^B = \delta^{AB} \tag{137}$$

(Klimeš 2002b, eq. 39). The simplest way of keeping condition (137) satisfied along the ray is to choose the derivatives of both vectors in the direction of ray–velocity vector $h_3^i = H^{,i}$,

$$\dot{\hat{h}}_i^A = -\frac{H^{,i}}{H^{,r} H^{,r}} \dot{h}_3^j \hat{h}_j^A \quad . \tag{138}$$

Inserting (68), we may express this equation in terms of the Hamiltonian,

$$\dot{\hat{h}}_i^A = -\frac{H^{,i}}{H^{,r}H^{,r}}(H^{,k}H^{,j}_{,k} - H_{,k}H^{,kj})\,\hat{h}_j^A \quad . \tag{139}$$

Note that the right–hand side of equation (139) is the ray–normal projection (with respect to the Cartesian metric) of the right–hand side of equation (145),

$$\dot{\hat{h}}_i^A = -\frac{H^{,i}H^{,k}}{H^{,r}H^{,r}}(H^{,j}_{,k} - p_k H_{,m}H^{,mj})\hat{h}_j^A \quad . \tag{140}$$

It is sufficient to calculate covariant basis vector $\hat{\mathbf{h}}^1$ by solving equation (139) numerically. Vector $\hat{\mathbf{h}}^2$ is then given by relation

$$\hat{\mathbf{h}}_2 = \frac{\mathbf{h}_3 \times \hat{\mathbf{h}}_1}{|\mathbf{h}_3 \times \hat{\mathbf{h}}_1|} \quad , \tag{141}$$

and contravariant vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ by relations (56) and (57).

The equation for the contravariant basis vectors may be obtained from (138) using relation (86),

$$\dot{h}_A^i = \left[(\dot{h}_3^i - H^{,i}p_k\dot{h}_3^k)\frac{H^{,j}}{H^{,r}H^{,r}} + H^{,i}H_{,j}\right]h_A^j \quad . \tag{142}$$

The 2×2 submatrix of 3×3 matrix (65) is

$$d_B^A = \frac{H^{,i}h_B^i}{H^{,r}H^{,r}}\dot{h}_3^j\hat{h}_j^A \quad . \tag{143}$$

This option requires the first and second derivatives of the Hamiltonian. When approaching isotropy, this ray–centred coordinate system with $w = \sqrt{H^{,i}H^{,i}}$ in (47) converges to the ray–centred coordinate system for isotropic media.

### 6.8. Basis vectors making $H^{(q),M}_{,N}$ zero

Klimeš (1994, 2002a, eqs. 52a and 52b) and Červený (2001, eq. 4.2.86) suggested the option making the mixed second derivatives (63) of the Hamiltonian in ray–centred coordinates zero,

$$\dot{h}_A^i = [H^{,i}_{,j} - (N-1)H^{,i}H_{,j}]h_A^j \quad , \tag{144}$$

$$\dot{\hat{h}}_i^A = -(H^{,j}_{,i} - p_i H_{,m}H^{,mj})\hat{h}_j^A \quad . \tag{145}$$

The 2×2 submatrix of the 3×3 matrix (65) is

$$d_B^A = \hat{h}_i^A H^{,i}_{,j} h_B^j \quad . \tag{146}$$

Similarly as the preceding option, this option requires the first and second derivatives of the Hamiltonian. Since no orthonormality relations between vectors $h_1^i$ and $h_2^i$ (or $\hat{h}_j^1$ and $\hat{h}_j^2$) are yet known, we would have to calculate both contravariant vectors (or both covariant vectors) by numerical integration. When approaching isotropy, this ray–centred coordinate system with $w = \sqrt{H^{,i}H^{,i}}$ in (47) converges to the ray–centred coordinate system for isotropic media.

## 7. Numerical implementation

### 7.1. Phase–space derivatives of the Hamiltonian

When calculating the homogeneous Hamiltonian of the second degree and its first and second phase–space derivatives, we first calculate the Christoffel matrix (1), its eigenvalues $G_{(a)}$ and eigenvectors $g_{i(a)}$. Then we calculate the P–wave Hamiltonian $\widetilde{H} = G_{(3)}$ or common S–wave Hamiltonian (36) with (28), and rescale the slowness vector according to the value of the Hamiltonian.

To calculate the first and second phase–space derivatives of the Christoffel matrix, transformed into the eigenvectors, we insert equations (2)–(6) into equations (19) and (20). The values of the density–reduced elastic moduli and the values of their first and second spatial derivatives are then multiplied by factors $g_{i(a)}g_{j(b)}p_m p_n$, $g_{i(a)}g_{j(b)}p_m$ or $g_{i(a)}g_{j(b)}$, which is numerically more efficient than to code equations (2)–(6) followed by transforms (19) and (20). In this way, we may calculate the second phase–space derivatives $\Gamma_{(aa),ij}$, $\Gamma_{(aa),i}^{\ \ ,j}$ and $\Gamma^{,ij}_{(aa)}$, and the first phase–space derivatives $\Gamma_{(ab),i}$ and $\Gamma^{,i}_{(ab)}$ with $(a) \neq (b)$. The first phase–space derivatives $\Gamma_{(aa),i}$ and $\Gamma^{,i}_{(aa)}$ may be calculated from $\Gamma_{(aa),i}^{\ \ ,j}$ and $\Gamma^{,ij}_{(aa)}$,

$$\Gamma_{(aa),i} = \tfrac{1}{2}\Gamma_{(aa),i}^{\ \ ,j} p_j \quad , \tag{147}$$

$$\Gamma^{,i}_{(ab)} = \Gamma^{,ij}_{(aa)} p_j \quad . \tag{148}$$

The first and second phase–space derivatives of the homogeneous P–wave Hamiltonian of the second degree are simply given by equations (22) and (23) with $(a) = (3)$. The first and second phase–space derivatives of the homogeneous S–wave Hamiltonian of degree $N$ are given by equations (29) and (31), with one of equations (32)–(35). The first and second phase–space derivatives of the homogeneous S–wave Hamiltonian of the second degree are then obtained from the first and second phase–space derivatives of the homogeneous S–wave Hamiltonian of degree $N$ using equations (37) and (38).

The calculation of the homogeneous Hamiltonian of the second degree and of its first and second phase–space derivatives has been coded and placed in new file "`hder.for`" of the Fortran 77 package MODEL (Bucha & Bulant 2003).

### 7.2. Modification of the "complete ray tracing" algorithm

In the following, we shall abbreviate the reference to the paper on the isotropic "complete ray tracing" algorithm (Červený, Klimeš & Pšenčík 1988) by ČKP.

For the modification of the isotropic complete ray tracing algorithm, we have selected options which are most similar to the original isotropic algorithm. In this way, the 4×4 paraxial ray propagator matrix is calculated by dynamic ray tracing in ray–centred coordinates, and the ray–centred coordinates are defined according to Section 6.6. The contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ are used in place of the isotropic basis vectors, because they have similar properties: $\mathbf{h}_1$ and $\mathbf{h}_2$ are unit vectors, perpendicular to the slowness vector, and mutually perpendicular (all with respect to the Cartesian metric).

The following modification of the quantities defined in the paper on isotropic complete ray tracing (ČKP) and calculated along the ray should be made for anisotropic media:

(a) Velocity $v$ (ČKP, eq. 5.1) used to parametrize the ray by a variable other than the travel time (e.g., by the arclength) is generalized to the ray velocity $v = \sqrt{H^{,i}H^{,i}}$.

(b) The isotropic basis vectors of the ray–centred coordinate system (ČKP, sec. 5.1.2 and quantities Y(9), Y(10) and Y(11) in sec. 5.2.1) are replaced by the contravariant basis vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ defined in Section 6.6.
(c) The isotropic basis vectors of the ray–centred coordinate system used as the polarization vectors (ČKP, sec. 5.1.4) should be replaced by the relevant eigenvectors of the Christoffel matrix. The great problem is to determine locally the S–wave eigenvectors in regions of close or identical S–wave velocities if the eigenvectors are not stored.
(d) P–wave and S–wave velocities stored at a point of the ray (ČKP, quantities YL(1) and YL(2) in sec. 5.5.4) are replaced by the phase velocities. Velocity gradient $v_{,i}$ (ČKP, quantities YL(4), YL(5) and YL(6) in sec. 5.5.4) is replaced by the spatial gradient of the Hamiltonian multiplied by the phase velocity, $v_{,i} = H_{,i}/\sqrt{p_m p_m}$.

Anisotropic P–wave ray tracing and anisotropic common S–wave ray tracing performed by program "`crt.for`" of the Fortran 77 package CRT is now applicable under the following restrictions:
(a) Only Cartesian coordinates are allowed.
(b) Only a smooth model without structural interfaces can be used, because the reference isotropic model is now used for the transformation at the interfaces (direction of the incident slowness vector is preserved but its norm is adjusted before transformation).
(c) No attenuation is considered with anisotropic ray tracing.
(d) There are no restrictions on the initial point, but if an initial line or initial surface is used, the initial travel time should be constant along the source.
(e) Dynamic ray tracing is not debugged.
Program "`green.for`" of the Fortran 77 package CRT has not been updated to consider anisotropic reference rays. Subroutine file "`ap.for`" has not been updated to consider correct polarization vectors in anisotropic media. Program "`invtt.for`" and subroutine file "`apvar.for`" of package CRT have not been updated to invert anisotropic travel times.

### 7.3. Numerical tests in models QI, QI2 and QI4

A vertically heterogeneous 1-D anisotropic model **QI** (model WA rotated through 45°) was provided by Pšenčík & Dellinger (2001) who performed the coupling ray theory calculations using the programs of package ANRAY (Pšenčík 1998) and compared the results with the anisotropic reflectivity calculations. The same model has been used by Bulant & Klimeš (2002a) and Klimeš & Bulant (2002) to demonstrate the coupling ray theory and its quasi–isotropic approximations. The data for model QI may be found on the compact disk by Bucha & Bulant (2003). For comparison with the isotropic and anisotropic ray theory seismograms in model QI and for a more detailed discussion and description of this model refer to Pšenčík & Dellinger (2001).

The density–normalized elastic moduli $a_{ijkl}$ at the surface (zero depth) are

$$\begin{array}{c c} & \begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \end{array} \\ \begin{array}{c} 11 \\ 22 \\ 33 \\ 23 \\ 13 \\ 12 \end{array} & \begin{pmatrix} 14.48500 & 4.52500 & 4.75000 & 0.00000 & 0.00000 & -0.58000 \\ & 14.48500 & 4.75000 & 0.00000 & 0.00000 & -0.58000 \\ & & 15.71000 & 0.00000 & 0.00000 & -0.29000 \\ & & & 5.15500 & -0.17500 & 0.00000 \\ & & & & 5.15500 & 0.00000 \\ & & & & & 5.04500 \end{pmatrix} \end{array} \qquad (149)$$

and at the depth of 1 length unit they are

$$
\begin{array}{c}
 \\ 11 \\ 22 \\ 33 \\ 23 \\ 13 \\ 12
\end{array}
\begin{array}{c}
\begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \end{array} \\
\begin{pmatrix}
22.08963 & 6.90063 & 7.24375 & 0.00000 & 0.00000 & -0.88450 \\
 & 22.08963 & 7.24375 & 0.00000 & 0.00000 & -0.88450 \\
 & & 23.95775 & 0.00000 & 0.00000 & -0.44225 \\
 & & & 7.86138 & -0.26688 & 0.00000 \\
 & & & & 7.86138 & 0.00000 \\
 & & & & & 7.69363
\end{pmatrix}
\end{array} \quad . \tag{150}
$$

The reference isotropic model is given by

$$v_{\rm P}^2 = 15.00 \quad , \qquad v_{\rm S}^2 = 5.10 \tag{151}$$

at the surface, and

$$v_{\rm P}^2 = 23.00 \quad , \qquad v_{\rm S}^2 = 7.79 \tag{152}$$

at the depth of 1 length unit. All the above values are interpolated linearly with depth. The homogeneous density is $\rho = 1$.

The differences of the elastic moduli of model **QI2** from the elastic moduli of the reference isotropic model (151), (152) are exactly twice larger than the differences of model QI. The density–normalized elastic moduli $a_{ijkl}$ of model QI2 at the surface (zero depth) are

$$
\begin{array}{c}
 \\ 11 \\ 22 \\ 33 \\ 23 \\ 13 \\ 12
\end{array}
\begin{array}{c}
\begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \end{array} \\
\begin{pmatrix}
13.97000 & 4.25000 & 4.70000 & 0.00000 & 0.00000 & -1.16000 \\
 & 13.97000 & 4.70000 & 0.00000 & 0.00000 & -1.16000 \\
 & & 16.42000 & 0.00000 & 0.00000 & -0.58000 \\
 & & & 5.21000 & -0.35000 & 0.00000 \\
 & & & & 5.21000 & 0.00000 \\
 & & & & & 4.99000
\end{pmatrix}
\end{array} \tag{153}
$$

and at the depth of 1 length unit they are

$$
\begin{array}{c}
 \\ 11 \\ 22 \\ 33 \\ 23 \\ 13 \\ 12
\end{array}
\begin{array}{c}
\begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \end{array} \\
\begin{pmatrix}
21.17926 & 6.38126 & 7.06750 & 0.00000 & 0.00000 & -1.76900 \\
 & 21.17926 & 7.06750 & 0.00000 & 0.00000 & -1.76900 \\
 & & 24.91550 & 0.00000 & 0.00000 & -0.88450 \\
 & & & 7.93276 & -0.53376 & 0.00000 \\
 & & & & 7.93276 & 0.00000 \\
 & & & & & 7.59726
\end{pmatrix}
\end{array} \quad . \tag{154}
$$

Analogously, the differences of the elastic moduli of model **QI4** from the elastic moduli of the reference isotropic model (151), (152) are exactly 4 times larger than the differences of model QI. The density–normalized elastic moduli $a_{ijkl}$ of model QI4 at the surface (zero depth) are

$$
\begin{array}{c}
 \\ 11 \\ 22 \\ 33 \\ 23 \\ 13 \\ 12
\end{array}
\begin{array}{c}
\begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \end{array} \\
\begin{pmatrix}
12.94000 & 3.70000 & 4.60000 & 0.00000 & 0.00000 & -2.32000 \\
 & 12.94000 & 4.60000 & 0.00000 & 0.00000 & -2.32000 \\
 & & 17.84000 & 0.00000 & 0.00000 & -1.16000 \\
 & & & 5.32000 & -0.70000 & 0.00000 \\
 & & & & 5.32000 & 0.00000 \\
 & & & & & 4.88000
\end{pmatrix}
\end{array} \quad . \tag{155}
$$

and at the depth of 1 length unit they are

$$\begin{array}{c} \\ 11 \\ 22 \\ 33 \\ 23 \\ 13 \\ 12 \end{array} \begin{array}{c} \begin{array}{cccccc} 11 & 22 & 33 & 23 & 13 & 12 \end{array} \\ \begin{pmatrix} 19.35852 & 5.34252 & 6.71500 & 0.00000 & 0.00000 & -3.53800 \\ & 19.35852 & 6.71500 & 0.00000 & 0.00000 & -3.53800 \\ & & 26.83100 & 0.00000 & 0.00000 & -1.76900 \\ & & & 8.07552 & -1.06752 & 0.00000 \\ & & & & 8.07552 & 0.00000 \\ & & & & & 7.40452 \end{pmatrix} \end{array} . \tag{156}$$

The point source is located at position $(50,50,0)^{\mathrm{T}}$, 29 receivers $(51,50,0.010)^{\mathrm{T}}$, $(51,50,0.030)^{\mathrm{T}}$, $(51,50,0.050)^{\mathrm{T}}$, ..., $(51,50,0.570)^{\mathrm{T}}$ are located in a vertical well.

The two–point anisotropic common S–wave rays have been traced from the point source to the receivers in models QI, QI2 and QI4 using homogeneous common S–wave Hamiltonian (28) of degree $N = -1$. The corresponding two–point anisotropic common S–wave travel times were then compared with the second–order travel–time perturbations from the two–point isotropic rays calculated in the isotropic reference model. The results of the comparison are shown in Tables 1, 2 and 3, for models QI, QI2 and QI4, respectively. The individual terms in the second–order perturbative Taylor expansion of the anisotropic common S–wave travel times in the vicinity of isotropic rays (Klimeš & Bulant 2002, eq. 17) are shown. Only the results at the $1^{\mathrm{st}}$, $8^{\mathrm{th}}$, $15^{\mathrm{th}}$, $22^{\mathrm{nd}}$ and $29^{\mathrm{th}}$ receivers are displayed, because the variation of the quantities along the vertical profile in models QI, QI2 and QI4 is very moderate.

## 8. Conclusions

The coupling ray theory for anisotropic media is now commonly applied to isotropic reference rays. Common S–wave ray tracing and the corresponding dynamic ray tracing will enable the coupling ray theory to be made more accurate, while preserving the comfort of common reference rays for both S–wave polarizations. For the comparison of errors of the coupling ray theory due to isotropic reference rays and due to anisotropic common S–wave reference rays refer to Klimeš & Bulant (2002, tables 1, 2 and 3).

The equations presented by Bakker (2002) and the equations presented in this paper are just a starting point. There still remain many tasks to be solved in order to put all advantages of common ray tracing to good use. For examples of the tasks refer to Section 8.1 below.

### 8.1. Future tasks

To test anisotropic P–wave and common S–wave ray tracing in other smooth models.

To debug anisotropic P–wave and common S–wave dynamic ray tracing in smooth models.

To code the anisotropic P–wave and common S–wave amplitudes in smooth models.

To derive and code the initial conditions for anisotropic P–wave and common S–wave amplitudes at point and linear sources.

To code the coupling ray theory Green tensor calculated along common S–wave reference rays, and the anisotropic ray theory Green tensor calculated along anisotropic P–wave rays.

To code the coupling ray theory Green tensor calculated along anisotropic S–wave reference rays.

| receiver depth | isotropic travel time | linear perturbation | quadratic perturbation | remaining difference | anisotropic travel time |
|---|---|---|---|---|---|
| 0.01 | 0.440990 | 0.000795 | 0.000062 | 0.000002 | 0.441850 |
| 0.15 | 0.438077 | 0.000742 | 0.000060 | 0.000000 | 0.438879 |
| 0.29 | 0.443550 | 0.000575 | 0.000059 | 0.000001 | 0.444184 |
| 0.43 | 0.456339 | 0.000328 | 0.000056 | -0.000001 | 0.456722 |
| 0.57 | 0.475206 | 0.000037 | 0.000052 | 0.000002 | 0.475297 |

**Table 1.** Comparison of anisotropic travel times, calculated along anisotropic common S–wave rays, with the second–order travel–time perturbations from isotropic rays in model QI.

| receiver depth | isotropic travel time | linear perturbation | quadratic perturbation | remaining difference | anisotropic travel time |
|---|---|---|---|---|---|
| 0.01 | 0.440990 | 0.003428 | 0.000258 | -0.000008 | 0.444668 |
| 0.15 | 0.438077 | 0.003309 | 0.000257 | -0.000009 | 0.441634 |
| 0.29 | 0.443550 | 0.002981 | 0.000261 | -0.000003 | 0.446788 |
| 0.43 | 0.456339 | 0.002500 | 0.000265 | -0.000010 | 0.459094 |
| 0.57 | 0.475206 | 0.001926 | 0.000266 | -0.000002 | 0.477395 |

**Table 2.** Comparison of anisotropic travel times, calculated along anisotropic common S–wave rays, with the second–order travel–time perturbations from isotropic rays in model QI2.

| receiver depth | isotropic travel time | linear perturbation | quadratic perturbation | remaining difference | anisotropic travel time |
|---|---|---|---|---|---|
| 0.01 | 0.440990 | 0.016117 | 0.001753 | -0.000287 | 0.458573 |
| 0.15 | 0.438077 | 0.015762 | 0.001797 | -0.000290 | 0.455345 |
| 0.29 | 0.443550 | 0.014971 | 0.001931 | -0.000279 | 0.460172 |
| 0.43 | 0.456339 | 0.013831 | 0.002101 | -0.000252 | 0.472020 |
| 0.57 | 0.475206 | 0.012452 | 0.002253 | -0.000195 | 0.489717 |

**Table 3.** Comparison of anisotropic travel times, calculated along anisotropic common S–wave rays, with the second–order travel–time perturbations from isotropic rays in model QI4.

**Tables 1, 2 and 3.** The *isotropic travel time* corresponds to a two–point ray traced in the reference isotropic model. The *linear perturbation* is the linear term in the perturbative Taylor expansion of the anisotropic common S–wave travel time in the vicinity of the isotropic ray according to Klimeš & Bulant (2002, eq. 17). The *quadratic perturbation* is the quadratic term in the perturbative Taylor expansion of the anisotropic common S–wave travel time in the vicinity of the isotropic ray. The *remaining difference* is the difference between the *anisotropic travel time*, corresponding to a two–point anisotropic common S–wave ray traced in the anisotropic model, and the second–order perturbative Taylor expansion in the vicinity of the isotropic ray (*isotropic travel time* + *linear perturbation* + *quadratic perturbation* + *remaining difference* = *anisotropic travel time*). The remaining difference accounts for the third–order and higher–order terms in the perturbative Taylor expansion and for numerical errors.

To test numerically the estimation of the travel–time error due to the common S–wave ray approximation.

To derive equations for the amplitude error due to the common S–wave ray approximation.

To code the initial conditions for anisotropic P–wave and common S–wave ray tracing and dynamic ray tracing for linear and surface sources.

To derive and code the transformation of anisotropic P–wave and common S–wave rays at structural interfaces between anisotropic media. To derive and code the corresponding transformations of ray–centred coordinate system, paraxial ray propagator matrix and amplitudes.

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