COMMON-RAY TRACING AND DYNAMIC RAY TRACING FOR S WAVES IN A SMOOTH ELASTIC ANISOTROPIC MEDIUM

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ABSTRACT

Anisotropic common S–wave rays are traced using the averaged Hamiltonian of both S–wave polarizations. They represent very practical reference rays for calculating S waves by means of the coupling ray theory. They eliminate problems with anisotropic–ray–theory ray tracing through some S–wave slowness–surface singularities and also considerably simplify the numerical algorithm of the coupling ray theory for S waves.

The equations required for anisotropic–common–ray tracing for S waves in a smooth elastic anisotropic medium, and for corresponding dynamic ray tracing in Cartesian or ray–centred coordinates, are presented. The equations, for the most part generally known, are summarized in a form which represents a complete algorithm suitable for coding and numerical applications.

Key words: travel time, ray tracing, dynamic ray tracing, geometrical spreading, S waves, coupling ray theory, seismic anisotropy, heterogeneous media

1. INTRODUCTION

The *coupling ray theory*, applicable to all degrees of anisotropy, from isotropic models to considerably anisotropic models, has been proposed by *Coates and 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 and Klimeš (2002)*.

It has been demonstrated that the coupling ray theory along *anisotropic–ray–theory reference rays* yields more accurate results for S waves than the anisotropic ray theory (*Bulant et al., 2004*; *Bulant and Klimeš, 2004*). Whereas tracing the continuous system of anisotropic–ray–theory rays may be very difficult in the vicinity of an S–wave slowness–surface singularity, at which the S–wave slowness surfaces coincide (*Vavryčuk, 2001, 2003*), this problem does not occur in the *common–ray approximation* for S waves. The common–ray approximation thus eliminates problems with anisotropic–ray–theory ray tracing through some S–wave slowness–surface singularities and also considerably simplifies 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 depend considerably on the degree of anisotropy and on the deviation of the reference ray path from the anisotropic–ray–theory ray paths.

In the commonly used *isotropic–common–ray approximation* (*Pšenčík, 1998*; *Pšenčík and Dellinger, 2001*), the isotropic–ray–theory rays are used as reference rays for the coupling ray theory, and isotropic–ray–theory geometrical spreading is used in approximating the scalar S–wave amplitude. *Bakker (2002)* proposed the *anisotropic–common–ray approximation*, in which the anisotropic common ray is traced using the averaged Hamiltonian of both S–wave polarizations. The anisotropic common rays then serve as reference rays for the coupling ray theory, and anisotropic–common–ray geometrical spreading is used in approximating the scalar S–wave amplitude. The anisotropic–common–ray approximation provides a better approximation of both travel times and amplitudes than the isotropic–common–ray approximation. *Klimeš and Bulant (2004)* estimated the travel–time errors due to the isotropic–common–ray and anisotropic–common–ray approximations using the second–order travel–time perturbations calculated along isotropic reference rays, and demonstrated the advantages of the anisotropic–common–ray approximation on a numerical example.

This paper is devoted to the equations required for tracing anisotropic common S–wave rays 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 useful for two–point ray tracing and for calculating amplitudes. We thus supplement the ray tracing equations with the equations for anisotropic common S–wave dynamic ray tracing, including the equations for the corresponding Hamiltonians and their first–order and second–order derivatives. Considerable attention is paid to dynamic ray tracing in ray–centred coordinates. All equations are expressed in a form suitable for numerical coding.

In Section 2, equations for the first–order and second–order partial phase–space derivatives of the eigenvalues of the Christoffel matrix for elastic waves are summarized. In Section 3, the anisotropic–ray-theory and anisotropic–common–ray Hamiltonians are introduced and equations for their first–order and second–order partial phase–space derivatives are presented. Note that equations (32)–(35) for regularizing the second–order partial phase–space derivatives of the anisotropic–common–ray Hamiltonian are necessary for robust dynamic ray tracing. Section 4 devoted to ray tracing and Section 5 devoted to dynamic ray tracing in ray–centred coordinates are applicable to a general Hamiltonian.

A common S–wave dynamic ray tracing algorithm based on the presented equations and suitable for modifying the isotropic "complete ray tracing" algorithm (*Červený et al., 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–ray tracing in a test example by *Bulant and Klimeš (2006)*, in which the two–point travel times calculated along anisotropic common rays have been compared with the second–order travel–time perturbations from isotropic rays, and vice versa. *Bulant and Klimeš (2006)* also estimated the travel–time errors due to the anisotropic–common–ray approximation using the second–order travel–time perturbations calculated along anisotropic common reference rays according to *Klimeš and Bulant (2006)*, and demonstrated the accuracy of the anisotropic–common–ray approximation on their numerical example.

As a by–product, this paper also contains the equations for anisotropic–ray–theory P–wave and S–wave ray tracing and dynamic ray tracing. The equations can thus be used to trace both anisotropic–ray–theory rays suitable for P waves and anisotropic common rays suitable for S waves.

The Einstein summation over the pairs of identical indices $a, b, c, ... = 1, 2, 3$ or $A, B, C, ... = 1, 2$ is used 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, e.g., $H_{,i} \equiv \partial H/\partial x^i$, $H^{,i} \equiv \partial H/\partial p_i$.

2. PARTIAL PHASE–SPACE DERIVATIVES OF THE EIGENVALUES OF THE CHRISTOFFEL MATRIX

The Christoffel matrix reads

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

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

As we need to handle both the derivatives with respect to x^m and p_n, we denote any partial phase–space derivative by $'$ or *. Both Γ'_{ij} and $\Gamma^\star_{ij}$ then stand for the first–order partial phase–space 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 partial phase–space 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*).

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

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

and

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

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),

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

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

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

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

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

Equation (13) may then be expressed as

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

equation (14) as

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

and equation (15) with (17) as

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

Equations (2)–(6), (19), (20), (22) and (23) are suitable for the numerical calculation of the first–order and second–order 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. Note that *Bakker (2002)* considered $N = 2$, whereas *Klimeš and Bulant (2004)* considered $N = -1$, which is better suited for travel–time perturbations as numerically demonstrated by *Bulant and Klimeš (2006, tables 7–12)*. 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 Hamiltonian $H(x^m, p_n)$, homogeneous with respect to slowness vector p_i.

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

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

its first–order partial phase–space derivatives are

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

and its second–order partial phase–space derivatives are

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

In the coupling ray theory, both S–wave polarizations are coupled. It is thus useful to have common reference rays equally suitable for both S–wave polarizations. For common–ray tracing, we shall thus consider the averaged Hamiltonian of both S–wave polarizations,

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

Note that we obtain different anisotropic common rays and different reference travel–time fields for different N. The first–order partial phase–space derivatives are

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

and the second–order partial phase–space derivatives are

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

We express the second–order derivatives of the common S–wave Hamiltonian in terms of the derivatives of the Christoffel matrix using equations (22) and (23),

$$\begin{aligned} H'^{\star} = {} & \frac{1}{4}\left[\Gamma'^{\star}_{(11)}(G_{(1)})^{\frac{N}{2}-1} + \Gamma'^{\star}_{(22)}(G_{(2)})^{\frac{N}{2}-1}\right] + \frac{\Gamma'_{(13)}\Gamma^{\star}_{(13)}(G_{(1)})^{\frac{N}{2}-1}}{2\,(G_{(1)} - G_{(3)})} + \frac{\Gamma'_{(23)}\Gamma^{\star}_{(23)}(G_{(2)})^{\frac{N}{2}-1}}{2\,(G_{(2)} - G_{(3)})} \\ & + \Gamma'_{(12)}\Gamma^{\star}_{(12)}\frac{(G_{(1)})^{\frac{N}{2}-1} - (G_{(2)})^{\frac{N}{2}-1}}{2\,(G_{(1)} - G_{(2)})} + \frac{N-2}{8}\left[\Gamma'_{(11)}\Gamma^{\star}_{(11)}(G_{(1)})^{\frac{N}{2}-2} + \Gamma'_{(22)}\Gamma^{\star}_{(22)}(G_{(2)})^{\frac{N}{2}-2}\right] . \end{aligned} \tag{31}$$

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–order phase–space derivatives of the Hamiltonian from Cartesian to ray centred coordinates depends on the degree N of the homogeneous Hamiltonian (*Klimeš, 2002*). 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–order partial phase–space derivatives are

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

and its second–order 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 $\widetilde{H} = \frac{1}{2}G_{(3)}$, $\widetilde{H}' = \frac{1}{2}G'_{(3)}$ and $\widetilde{H}'^{\star} = \frac{1}{2}G'^{\star}_{(3)}$.

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

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

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

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

$$\dot{\tau} = H^{,k} p_k = 1 \quad . \tag{41}$$

The dot then represents the derivative with respect to travel time τ along the ray.

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 γ,

$$\dot{Q}^i = H^{,i}_{,j} Q^j + H^{,ij} P_j \quad , \tag{42}$$

$$\dot{P}_i = -H_{,ij} Q^j - H^{,j}_{,i} P_j \quad , \tag{43}$$

where

$$Q^i = \frac{\partial x^i}{\partial \gamma} \quad , \tag{44}$$

$$P_i = \frac{\partial p_i}{\partial \gamma} \quad . \tag{45}$$

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 *Popov and Pšenčík (1978a, 1978b)*, and then to dynamic ray tracing in anisotropic media by *Hanyga (1982)*, *Kendall et al. (1992)* and *Klimeš (1994)*.

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

$$q^3 = q_0^3 + \int_{\tau_0}^{\tau} w \, \mathrm{d}\tau \quad . \tag{46}$$

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, $w = \sqrt{H^{,i} H^{,i}}$. In this paper, 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 dynamic ray tracing. We shall thus put $w = 1$.

The q^A coordinates lie, for fixed q^3, in the wavefront tangent plane. The Cartesian coordinates corresponding to q^m are

$$x^i = x_0^i(q^3) + h_M^i(q^3) \, q^M \quad , \tag{47}$$

where $x_0^i(q^3)$ 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

$$h_m^i = \frac{\partial x^i}{\partial q^m} \quad , \qquad \hat{h}_i^m = \frac{\partial q^m}{\partial x^i} \quad . \tag{48}$$

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*)

$$h_3^i = H^{,i} \quad , \tag{49}$$

$$\hat{h}_i^3 = p_i \quad , \tag{50}$$

$$h_a^i \hat{h}_i^b = \delta_a^b \quad . \tag{51}$$

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 (49) and (50), 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 $\mathbf{h}_2$ are known, the covariant basis vectors $\hat{\mathbf{h}}^1$ and $\hat{\mathbf{h}}^2$ are given by relations

$$\hat{\mathbf{h}}^1 = \frac{\mathbf{h}_3 \times \mathbf{h}_2}{\mathbf{h}_1^{\mathrm{T}} (\mathbf{h}_3 \times \mathbf{h}_2)} \quad , \tag{52}$$

$$\hat{\mathbf{h}}^2 = \frac{\mathbf{h}_3 \times \mathbf{h}_1}{\mathbf{h}_2^{\mathrm{T}}\,(\mathbf{h}_3 \times \mathbf{h}_1)} \quad . \tag{53}$$

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

$$\mathbf{h}_1 = \frac{\mathbf{p} \times \hat{\mathbf{h}}^2}{\hat{\mathbf{h}}_1^{\mathrm{T}}\,(\mathbf{p} \times \hat{\mathbf{h}}^2)} \quad , \tag{54}$$

$$\mathbf{h}_2 = \frac{\mathbf{p} \times \hat{\mathbf{h}}^1}{\hat{\mathbf{h}}_2^{\mathrm{T}}\,(\mathbf{p} \times \hat{\mathbf{h}}^1)} \quad . \tag{55}$$

The 4×4 dynamic ray tracing system in ray–centred coordinates reads (*Klimeš, 1994, eq. 60*)

$$\dot{Q}^M_{(q)} = H^{(q),M}_{,N} Q^N_{(q)} + H^{,MN}_{(q)} P^{(q)}_N \quad , \tag{56}$$

$$\dot{P}^{(q)}_M = -H^{(q)}_{,MN} Q^N_{(q)} - H^{(q),N}_{,M} P^{(q)}_N \quad , \tag{57}$$

where

$$Q^M_{(q)} = \frac{\partial q^M}{\partial \gamma} \quad , \tag{58}$$

$$P^{(q)}_M = \frac{\partial}{\partial \gamma}\left(\frac{\partial \tau}{\partial q^M}\right) \quad . \tag{59}$$

The second–order 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*; *Klimeš, 2002, eqs. 51a, 51b, 51c*)

$$H^{(q)}_{,AB} = h^j_A [H_{,jk} - (N-1) H_{,j} H_{,k}] h^k_B \quad , \tag{60}$$

$$H^{(q),N}_{,M} = h^j_M H_{,j}^{,k} \hat{h}^N_k - d^N_M \quad , \tag{61}$$

$$H^{,MN} = \hat{h}^M_j H^{,jk} \hat{h}^N_k \quad . \tag{62}$$

The four coefficients

$$d^N_M = \hat{h}^N_i \dot{h}^i_M = -h^i_M \dot{\hat{h}}^N_i \tag{63}$$

in equation (61) 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 is discussed in detail by *Klimeš (2006)*. On the other hand, the choice of the four coefficients d^N_M uniquely determines 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 (*Klimeš, 2006*).

6. NUMERICAL IMPLEMENTATION

6.1. Phase–space derivatives of the Hamiltonian

When calculating the homogeneous Hamiltonian of the second degree and its first–order and second–order phase–space derivatives, we first calculate Christoffel matrix (1), its eigenvalues $G_{(a)}$ and eigenvectors $g_{i(a)}$. We then 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–order and second–order 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–order and second–order spatial derivatives are 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 calculate the second–order phase–space derivatives $\Gamma_{(aa),ij}$, $\Gamma_{(aa),i}{}^{,j}$ and $\Gamma_{(aa)}^{,ij}$, and the first–order phase–space derivatives $\Gamma_{(ab),i}$ and $\Gamma_{(ab)}^{,i}$ with $(a) \neq (b)$. The first–order phase–space derivatives $\Gamma_{(aa),i}$ and $\Gamma_{(aa)}^{,i}$ can be calculated from $\Gamma_{(aa),i}{}^{,j}$ and $\Gamma_{(aa)}^{,ij}$,

$$\Gamma_{(aa),i} = \tfrac{1}{2}\Gamma_{(aa),i}{}^{,j} p_j \quad , \tag{64}$$

$$\Gamma_{(aa)}^{,i} = \Gamma_{(aa)}^{,ij} p_j \quad . \tag{65}$$

The first–order and second–order 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–order and second–order phase–space derivatives of the homogeneous common S–wave Hamiltonian of degree N are given by equations (29) and (31), with one of the equations (32)–(35). The first–order and second–order phase–space derivatives of the homogeneous common S–wave Hamiltonian of the second degree are then obtained from the first–order and second–order phase–space derivatives of the homogeneous common 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–order and second–order phase–space derivatives has been coded and placed in file "`hder.for`" of the Fortran 77 package MODEL (*Bucha and Bulant, 2003*).

6.2. Modification of the isotropic ray tracing algorithm

For the modification of the isotropic "complete ray tracing" algorithm by *Červený et al. (1988)*, 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 according to Section 5, and the ray–centred coordinates are defined according to *Klimeš (2006, sec. 5.4)*. This ray–centred coordinate system represents one of the various possible generalizations of the ray–centred coordinate system for isotropic media by *Popov and Pšenčík (1978a,* *1978b)*. 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).

Anisotropic–ray–theory ray tracing for P waves and anisotropic–common–ray tracing for S waves in smooth anisotropic models without interfaces and corresponding dynamic ray tracing in ray–centred coordinates have been coded, added to the Fortran 77 CRT package, debugged and numerically tested (*Bucha and Bulant, 2004*; *Bulant and Klimeš, 2006*). For the numerical example of anisotropic–common–ray tracing and for the application of the numerical algorithm of the coupling ray theory by *Bulant and Klimeš (2002)* along anisotropic common S–wave rays refer to *Bulant and Klimeš (2006)*.

7. CONCLUSIONS

The coupling ray theory for S waves in anisotropic media has recently been applied to isotropic reference rays (*Pšenčík, 1998*; *Pšenčík and Dellinger, 2001*). The equations presented by *Bakker (2002)* and the equations presented in this paper allow anisotropic common S–wave reference rays to be traced. Common–ray tracing for S waves and corresponding dynamic ray tracing enable the coupling ray theory to be made more accurate, while preserving the comfort of common reference rays for both S–wave polarizations. The anisotropic common rays also eliminate problems with anisotropic–ray–theory ray tracing through some S–wave slowness–surface singularities.

The equations of this paper represent a complete algorithm suitable for anisotropic–common–ray tracing for S waves in a smooth elastic anisotropic medium, and for corresponding dynamic ray tracing in Cartesian or ray–centred coordinates. For the comparison of travel–time errors of the coupling ray theory due to isotropic reference rays and due to anisotropic common S–wave reference rays refer to *Bulant and Klimeš (2006, tables 4–9)*.

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

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