Transformations for dynamic ray tracing in anisotropic media with a homogeneous Hamiltonian of an arbitrary degree

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Summary

Six–dimensional dynamic ray tracing in (phase–space) Cartesian coordinates was introduced by Červený in 1972. In 1982, Hanyga showed that it reduces to 4–dimensional dynamic ray tracing in (phase–space) ray–centred coordinates. This paper concentrates on the explicit transformation equations of dynamic ray tracing between Cartesian and ray–centred coordinates. Many of the transformation equations have not been published before even for isotropic medium. Also proposed is an efficient way of reducing the number of equations being solved when numerically evaluating the paraxial–ray propagator matrices, both in Cartesian and ray–centred coordinates.

Key words

Anisotropy, paraxial rays, dynamic ray tracing, ray–centred coordinates.

1. Introduction

Dynamic ray tracing consists in the solution of a system of ordinary differential equations along a ray. It yields the first derivatives of phase-space coordinates of a point of the ray with respect to initial conditions. It is of particular importance when calculating second and higher spatial travel-time derivatives, when calculating ray perturbations with respect to initial conditions or model variations, for two-point ray tracing, for the paraxial ray approximation, for computing paraxial Gaussian beams and packets, etc.

The dynamic ray tracing equations in anisotropic media were derived in Cartesian coordinates by Červený (1972). The results of Červený's paper are not reviewed here. In particular, equations for the eigenvalues G of the Christoffel matrix (5) and their first and second derivatives with respect to Cartesian coordinates, necessary for numerical applications, can be found in Červený's paper.

Ray–centred coordinates are defined in terms of a given axial ray and the corresponding wavefront tangent planes. Ray–centred coordinates were used by Luneburg (1944, Sec.12) for the polarization of electromagnetic waves in isotropic media, and by Popov & Pšenčík (1978a,b) for both dynamic ray tracing and polarization of elastic waves in isotropic media, then generalized for anisotropic media by Hanyga (1982) and Kendall, Guest & Thomson (1992). In this paper we follow the approach of the latter paper.

In this paper, the main attention is devoted to the transformation relations of dynamic ray tracing between Cartesian and ray–centred coordinates. The results achieved may be used to compare the equations derived alternately in both the coordinate systems, to transform the equations from one coordinate system to the other, to transform

In: Seismic Waves in Complex 3-D Structures, Report 12 (Department of Geophysics, Charles University, Prague, 2002), pp. 67–78.
The version with a homogeneous Hamiltonian of the second degree was published previously in Wave Motion, **20** (1994), 261–272.
The differences between the two versions are marked with red.

the outcomes of numerical calculations from one coordinate system to the other, and to calculate the whole 6×6 paraxial ray propagator matrix in a very efficient way. All equations are, of course, also applicable in isotropic media.

2. Anisotropic ray theory

Assume the anisotropic elastodynamic equation for vector u_k in orthonormal Cartesian coordinates x^m, expressed as

$$\frac{\partial}{\partial x^i}\left(c^{ijkl}\frac{\partial}{\partial x^l}u_k\right)=\rho\frac{\partial^2}{\partial t^2}u_j \quad , \tag{1}$$

where t is time, $c^{ijkl}=c^{ijkl}(x^m)$ and $\rho=\rho(x^m)$ are time–independent material parameters. For instance, in the case of elastic waves, $c^{ijkl}=c^{ijkl}(x^m)$ are the elastic parameters, $\rho=\rho(x^m)$ is the density, and $u_j=u_j(x^m)$ are the components of the displacement vector. For the definition and discussion of Cartesian coordinates see Appendix A. In this paper, we shall assume that the seismic model is prescribed in orthonormal Cartesian coordinates, and that the rays are traced in Cartesian coordinates. For other coordinate systems, refer to Appendix B.

The solution of (1) is sought in the form of a ray series

$$u_k(x^m,t)=\sum_{\nu=0}^{\infty}U_k^{(\nu)}(x^m)\ f^{(\nu)}\Big(t-\tau(x^n)\Big) \quad , \tag{2}$$

where functions $f^{(\nu)}(\vartheta)$ satisfy the relation

$$\tfrac{\mathrm{d}}{\mathrm{d}\vartheta}f^{(\nu+1)}(\vartheta)=f^{(\nu)}(\vartheta), \quad \nu=-2,-1,0,1,2,... \quad . \tag{3}$$

After substituting (2) into (1), the terms with the highest order of discontinuity, containing $f^{(-2)}$, yield the equation

$$\Gamma^{jk}U_k^{(0)}=U_j^{(0)} \quad , \tag{4}$$

where

$$\Gamma^{jk}=\tfrac{\partial\tau}{\partial x^i}\ c^{ijkl}\ \tfrac{\partial\tau}{\partial x^l}\ \rho^{-1} \tag{5}$$

is the *Christoffel matrix.* The wave polarization is thus given by an eigenvector of the Christoffel matrix, and travel time $\tau(x^n)$ has to satisfy the *eikonal equation*

$$G(x^m,\tfrac{\partial\tau}{\partial x^m})=1 \quad , \tag{6}$$

where G is the corresponding eigenvalue. For more details refer to Červený (1972).

3. Phase–space coordinates

The slowness vector components corresponding to coordinates x^i are

$$p_i^{(x)} = \frac{\partial \tau}{\partial x^i} \quad , \tag{7}$$

where τ is the travel time. The corresponding coordinates in phase space are

$$w_{(x)}^{\underline{i}} = \begin{pmatrix} w_{(x)}^{i} \\ w_i^{(x)} \end{pmatrix} = \begin{pmatrix} x^i \\ p_i^{(x)} \end{pmatrix} \quad . \tag{8}$$

The underlined lower–case superscript ($w^{\underline{i}}$) takes six values: first the values 1,2,3 as superscript (w^i), then the same set of values as subscript (w_i). The underlined upper–case superscript ($W^{\underline{N}}$) takes four values: 1,2 as superscript (W^N), then 1,2 as subscript (W_N). Similarly, the underlined subscript ($H_{\underline{i}}$) first takes the subscript values (H_i), then the superscript values (H^i). Thus, the underlined index takes twice the number of values that would be taken were it not underlined.

Now, eigenvalue G of the Christoffel matrix (5) may be viewed as a function of phase-space coordinates, $G = G\,(x^m, p_m^{(x)})$.

4. Ray tracing

We define the Hamiltonian as

$$H = \tfrac{1}{N} G^{\frac{N}{2}} \quad , \tag{9}$$

where G is the eigenvalue of the Christoffel matrix, corresponding to the polarization under consideration, see eikonal equation (6). Note that the Hamiltonian may be introduced in many other forms, yielding independent variables along a ray other than the travel time (Kendall & Thomson 1989). However, in this paper we prefer this kind of Hamiltonian, assuming that the independent variable along a ray is the travel time. Introducing the gradient of the Hamiltonian in phase space,

$$H_{\underline{i}}^{(x)} = \begin{pmatrix} H_i^{(x)} \\ H_{(x)}^i \end{pmatrix} = \frac{\partial H}{\partial w_{(x)}^{\underline{i}}} = \begin{pmatrix} \frac{\partial H}{\partial x^i} \\ \frac{\partial H}{\partial p_i^{(x)}} \end{pmatrix} \quad , \tag{10}$$

the ray-tracing equations may be expressed in the concise form of

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau} w_{(x)}^{\underline{i}} = \Sigma^{\underline{ij}} H_{\underline{j}}^{(x)} \quad , \tag{11}$$

where $\Sigma^{\underline{ij}}$ are components of the 6×6 matrix

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \quad , \tag{12}$$

with $\mathbf{0}$ and $\mathbf{1}$ being 3×3 zero and identity matrices.

5. Isotropic medium

All equations are also valid in an isotropic medium, in which

$$H = \tfrac{1}{N} G^{\frac{N}{2}} = \tfrac{1}{N} v^N [p_i g^{ij} p_j]^{\frac{N}{2}} \quad , \tag{13}$$

where $v = v(x^m)$ is the propagation velocity, and g^{ij} is the Cartesian metric tensor, an identity matrix in orthonormal Cartesian coordinates.

6. Dynamic ray tracing

The phase–space coordinates (8) of the initial points of rays are the initial conditions for the ray tracing equations (11). In a 6–dimensional phase space, these initial conditions may be functions of up to 6 locally independent ray parameters. Let us consider a one–parametric subsystem of rays, parametrized by γ. Parameter γ is generally one of several ray parameters, arbitrarily selected. The partial derivative with respect to γ is taken for the other ray parameters fixed, and for fixed parameter τ along the ray.

We introduce the paraxial–ray phase–space coordinates

$$W^{\underline{i}}_{(x)} = \begin{pmatrix} Q^i_{(x)} \\ P^{(x)}_i \end{pmatrix} = \frac{\partial}{\partial\gamma} w^{\underline{i}}_{(x)} = \frac{\partial}{\partial\gamma} \begin{pmatrix} x^i \\ p^{(x)}_i \end{pmatrix} \quad . \tag{14}$$

Since the phase–space coordinates (8) are functions of the ray parameters and of parameter τ along the ray, $\frac{\partial}{\partial\gamma}$ commutes with $\frac{\mathrm{d}}{\mathrm{d}\tau}$. Differentiating the ray tracing equations (11) with respect to γ, we arrive at the dynamic ray tracing equations

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau} W^{\underline{i}}_{(x)} = \Sigma^{\underline{i}\underline{j}} H^{(x)}_{\underline{j}\underline{k}} W^{\underline{k}}_{(x)} \quad . \tag{15}$$

Here

$$\mathbf{H}^{(x)} = \begin{pmatrix} \mathbf{H}^{(x)}_{\bullet\bullet} & \mathbf{H}^{(x)\bullet}_{\bullet} \\ \mathbf{H}^{\bullet}_{(x)\bullet} & \mathbf{H}^{\bullet\bullet}_{(x)} \end{pmatrix} \tag{16}$$

is the 6×6 matrix of the second phase–space partial derivatives of the Hamiltonian,

$$H^{(x)}_{\underline{i}\underline{k}} = \begin{pmatrix} H^{(x)}_{ik} & H^{(x)k}_{i} \\ H^{i}_{(x)k} & H^{ik}_{(x)} \end{pmatrix} = \frac{\partial^2 H}{\partial w^{\underline{i}}_{(x)} \partial w^{\underline{k}}_{(x)}} = \begin{pmatrix} \frac{\partial^2 H}{\partial x^i \partial x^k} & \frac{\partial^2 H}{\partial x^i \partial p^{(x)}_k} \\ \frac{\partial^2 H}{\partial p^{(x)}_i \partial x^k} & \frac{\partial^2 H}{\partial p^{(x)}_i \partial p^{(x)}_k} \end{pmatrix} \quad . \tag{17}$$

We have introduced the above notation for the partial derivatives of H in order to avoid complicated indices. Instead of employing subscripts and superscripts, many authors use alternative notations such as $H^{(x)}_{x^i x^k} = H^{(x)}_{ik}$, $H^{(x)}_{x^i p^{(x)}_k} = H^{(x)k}_{i}$, $H^{(x)}_{p^{(x)}_i x^k} = H^{i}_{(x)k}$, $H^{(x)}_{p^{(x)}_i p^{(x)}_k} = H^{ik}_{(x)}$, etc.

Note that the Hamiltonian is a homogeneous function of $p^{(x)}_i$ of the Nth degree (Červený 1972),

$$H^{i}_{(x)} p^{(x)}_i = NH = 1 \quad . \tag{18}$$

Consequently,

$$H^{ij}_{(x)} p^{(x)}_j = (N{-}1) H^{i}_{(x)} \quad . \tag{19}$$

In determining the ray as a geodesic in curved space, matrix components $H^{ik}_{(x)}$ for $N=2$ are the contravariant components of the corresponding Finslerian metric tensor. Thus, we may call matrix $H^{ik}_{(x)}$ for $N=2$ the *wave–propagation metric tensor*. In the case of electromagnetic waves, the wave–propagation metric tensor is closely related to the metric tensor of the general theory of relativity.

7. Ray–centred coordinates

The q^3–coordinate line of ray–centred coordinates q^m is the axial ray. The q^A coordinates lie, for fixed q^3, in the wavefront tangent plane (Hanyga 1982; Kendall *et al.* 1992), $q^3 = \tau$. The Cartesian coordinates corresponding to q^m are

$$x^i = x^i_0(q^3) + h^i{}_M(q^3)\, q^M \quad , \tag{20}$$

where $x^i_0(\tau)$ 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. Basis vectors $h^i{}_M(\tau)$ are chosen arbitrarily in the wavefront tangent plane,

$$p_i\, h^i{}_M = 0 \quad . \tag{21}$$

The transformation matrices, taken at the central ray, are

$$h^i{}_m = \frac{\partial x^i}{\partial q^m} \quad , \qquad \hat{h}^m{}_i = \frac{\partial q^m}{\partial x^i} \quad , \tag{22}$$

where

$$\hat{h}^3{}_i = p^{(x)}_i \quad , \qquad h^i{}_3 = H^i_{(x)} \quad , \qquad \hat{h}^m{}_i h^i{}_n = \delta^m_n \quad , \qquad h^i{}_m \hat{h}^m{}_j = \delta^i_j \quad . \tag{23}$$

As in any coordinates, the dynamic ray tracing equations (15) are also valid in ray–centred coordinates,

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau} W^{\underline{i}}_{(q)} = \Sigma^{\underline{ij}} H^{(q)}_{\underline{jk}} W^{\underline{k}}_{(q)} \quad . \tag{24}$$

Here the notation is analogous to that in Cartesian coordinates,

$$p^{(q)}_i = \frac{\partial \tau}{\partial q^i} \quad , \tag{25}$$

$$w^{\underline{i}}_{(q)} = \begin{pmatrix} w^i_{(q)} \\ w^{(q)}_i \end{pmatrix} = \begin{pmatrix} q^i \\ p^{(q)}_i \end{pmatrix} \quad , \tag{26}$$

$$W^{\underline{i}}_{(q)} = \begin{pmatrix} Q^i_{(q)} \\ P^{(q)}_i \end{pmatrix} = \frac{\partial}{\partial \gamma} w^{\underline{i}}_{(q)} = \frac{\partial}{\partial \gamma} \begin{pmatrix} q^i \\ p^{(q)}_i \end{pmatrix} \quad , \tag{27}$$

$$H^{(q)}_{\underline{ik}} = \begin{pmatrix} H^{(q)}_{ik} & H^{(q)\,k}_i \\ H^i_{(q)\,k} & H^{ik}_{(q)} \end{pmatrix} = \frac{\partial^2 H}{\partial w^{\underline{i}}_{(q)} \partial w^{\underline{k}}_{(q)}} = \begin{pmatrix} \frac{\partial^2 H}{\partial q^i \partial q^k} & \frac{\partial^2 H}{\partial q^i \partial p^{(q)}_k} \\ \frac{\partial^2 H}{\partial p^{(q)}_i \partial q^k} & \frac{\partial^2 H}{\partial p^{(q)}_i \partial p^{(q)}_k} \end{pmatrix} \quad . \tag{28}$$

Equations (24), (25), (26), (27), and (28) are just the ray–centred coordinate versions of equations (15), (7), (8), (14), and (17).

8. Transformation

8.1 Transformation of the paraxial–ray phase–space coordinates

The transformation equations for the paraxial–ray phase–space coordinates from the Cartesian to ray–centred coordinate system read

$$Q^m_{(q)} = \frac{\partial q^m}{\partial \gamma} = \frac{\partial q^m}{\partial x^i}\frac{\partial x^i}{\partial \gamma} = \hat{h}^m{}_i Q^i_{(x)} \quad , \tag{29}$$

$$\begin{aligned} P^{(q)}_m &= \frac{\partial}{\partial \gamma}\frac{\partial \tau}{\partial q^m} = \frac{\partial}{\partial \gamma}\left(\frac{\partial \tau}{\partial x^i}\frac{\partial x^i}{\partial q^m}\right) \\ &= \frac{\partial x^i}{\partial q^m}\frac{\partial}{\partial \gamma}\frac{\partial \tau}{\partial x^i} + \frac{\partial \tau}{\partial x^i}\frac{\partial^2 x^i}{\partial q^m \partial q^n}\frac{\partial q^n}{\partial \gamma} = h^i{}_m P^{(x)}_i + p^{(x)}_i \frac{\partial^2 x^i}{\partial q^m \partial q^n} Q^n_{(q)} \quad . \end{aligned} \tag{30}$$

It may be convenient to introduce matrices

$$\bar{Q}^m_{(q)} = \hat{h}^m{}_i Q^i_{(x)} \quad , \qquad \bar{P}^{(q)}_m = h^i{}_m P^{(x)}_i \quad , \tag{31a}$$

or, concisely,

$$\bar{W}^{\underline{m}}_{(q)} = \hat{h}^{\underline{m}}{}_{\underline{i}} W^{\underline{i}}_{(x)} \quad , \tag{31b}$$

where

$$\hat{h}^{\underline{m}}{}_{\underline{i}} = \begin{pmatrix} \hat{h}^m{}_i & 0^{mi} \\ 0_{mi} & h^i{}_m \end{pmatrix} \quad , \tag{32}$$

0^{kl} and 0_{kl} being zeros. Matrices $\bar{Q}^m_{(q)}$ and $\bar{P}^{(q)}_m$ are the covariant versions of $Q^m_{(q)}$ and $P^{(q)}_m$, i.e. they are defined by an equation similar to (27) with the partial derivative with respect to γ replaced by the covariant derivative. Here the word "covariant" is again understood in the sense of the Cartesian metric. In other words, $\bar{Q}^m_{(q)}$ and $\bar{P}^{(q)}_m$ are matrices similar to $Q^m_{(x)}$, $P^{(x)}_m$ or $Q^m_{(q)}$, $P^{(q)}_m$, but defined with respect to the local Cartesian coordinates connected with the basis vectors of the ray–centred coordinate system. Substituting the word "partial" by the word "covariant" only means locally substituting curvilinear coordinates by the Cartesian coordinates with the same basis vectors. Then

$$Q^m_{(q)} = \bar{Q}^m_{(q)} \quad , \qquad P^{(q)}_m = \bar{P}^{(q)}_m + F_{mn}\bar{Q}^n_{(q)} \quad , \tag{33a}$$

or, concisely,

$$W^{\underline{m}}_{(q)} = F^{\underline{m}}{}_{\underline{n}} \bar{W}^{\underline{n}}_{(q)} \quad , \tag{33b}$$

where

$$F_{mn} = p^{(x)}_i \frac{\partial^2 x^i}{\partial q^m \partial q^n} \tag{34}$$

and

$$F^{\underline{m}}{}_{\underline{n}} = \begin{pmatrix} \delta^m{}_n & 0^{mn} \\ F_{mn} & \delta_m{}^n \end{pmatrix} \quad . \tag{35}$$

Equations (20), (23), and (11) yield

$$F_{MN} = 0 \quad , \qquad F_{m3} = F_{3m} = p^{(x)}_i \tfrac{\mathrm{d}}{\mathrm{d}\tau} h^i{}_m = -h^i{}_m \tfrac{\mathrm{d}}{\mathrm{d}\tau} p^{(x)}_i = h^i{}_m H^{(x)}_i = H^{(q)}_m \quad . \tag{36}$$

The inverse transform to (31a,b) is

$$Q^i_{(x)} = h^i{}_m \bar{Q}^m_{(q)} \quad , \qquad P^{(x)}_i = \hat{h}^m{}_i \bar{P}^{(q)}_m \quad , \tag{37a}$$

or, concisely,

$$W^{\underline{i}}_{(x)} = h^{\underline{i}}{}_{\underline{m}} \bar{W}^{\underline{m}}_{(q)} \quad , \tag{37b}$$

where

$$h^{\underline{i}}{}_{\underline{m}} = \begin{pmatrix} h^i{}_m & 0^{im} \\ 0_{im} & \hat{h}^m{}_i \end{pmatrix} \tag{38}$$

is inverse matrix to (32). The inverse transform to (33a,b) is

$$\bar{Q}^m_{(q)} = Q^m_{(q)} \quad , \qquad \bar{P}^{(q)}_m = P^{(q)}_m - F_{mn} Q^n_{(q)} \quad , \tag{39a}$$

or, concisely,

$$\bar{W}^{\underline{m}}_{(q)} = \hat{F}^{\underline{m}}{}_{\underline{n}} W^{\underline{n}}_{(q)} \quad , \tag{39b}$$

where

$$\hat{F}^{\underline{m}}{}_{\underline{n}} = \begin{pmatrix} \delta^m{}_n & 0^{mn} \\ -F_{mn} & \delta_m{}^n \end{pmatrix} \tag{40}$$

is inverse matrix to (35).

8.2 The second Hamiltonian derivatives in the local Cartesian coordinates

Inserting (37b) into (15), we arrive at the version

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \bar{W}^{\underline{i}}_{(q)} = \Sigma^{\underline{i}\underline{j}} \bar{H}^{(q)}_{\underline{j}\underline{k}} \bar{W}^{\underline{k}}_{(q)} \tag{41}$$

of the dynamic ray tracing system, where

$$\bar{H}^{(q)}_{\underline{m}\underline{n}} = -\Sigma^{\underline{m}\underline{l}} \hat{h}^{\underline{l}}{}_{\underline{i}} \left(\Sigma^{\underline{i}\underline{j}} H^{(x)}_{\underline{j}\underline{k}} h^{\underline{k}}{}_{\underline{n}} - \frac{\mathrm{d}}{\mathrm{d}\tau} h^{\underline{i}}{}_{\underline{n}} \right) = h^{\underline{j}}{}_{\underline{m}} H^{(x)}_{\underline{j}\underline{k}} h^{\underline{k}}{}_{\underline{n}} + \Sigma^{\underline{m}\underline{l}} \hat{h}^{\underline{l}}{}_{\underline{i}} \frac{\mathrm{d}}{\mathrm{d}\tau} h^{\underline{i}}{}_{\underline{n}} \quad . \tag{42}$$

The 3×3 submatrices of (42) are

$$\bar{H}^{(q)}_{mn} = h^j{}_m H^{(x)}_{jk} h^k{}_n \quad , \tag{43a}$$

$$\bar{H}^{(q)\,n}_m = \bar{H}^{n}_{(q)\,m} = h^j{}_m H^{(x)\,k}_j \hat{h}^n{}_k + h^i{}_m \frac{\mathrm{d}}{\mathrm{d}\tau} \hat{h}^n{}_i = h^j{}_m H^{(x)\,k}_j \hat{h}^n{}_k - \hat{h}^n{}_i \frac{\mathrm{d}}{\mathrm{d}\tau} h^i{}_m \quad , \tag{43b}$$

$$\bar{H}^{mn}_{(q)} = \hat{h}^m{}_j H^{jk}_{(x)} \hat{h}^n{}_k \quad . \tag{43c}$$

In view of (11), (18), (19), and (23),

$$\bar{H}^{(q)\,3}_m = N h^j{}_m H^{(x)}_j - h^i{}_m H^{(x)}_i = (N{-}1) H^{(q)}_m \quad , \tag{44a}$$

$$\bar{H}^{(q)\,m}_3 = H^j_{(x)} H^{(x)\,k}_j \hat{h}^m{}_k - \hat{h}^m{}_i \frac{\mathrm{d}}{\mathrm{d}\tau} H^i_{(x)} = H^{(x)}_j H^{jk}_{(x)} \hat{h}^m{}_k \quad , \tag{44b}$$

$$\bar{H}^{M3}_{(q)} = \bar{H}^{3M}_{(q)} = 0 \quad , \qquad \bar{H}^{33}_{(q)} = N(N{-}1)H = N{-}1 \quad . \tag{44c}$$

8.3 The second Hamiltonian derivatives in the ray–centred coordinates

Inserting (39b) into (41) we arrive at (24), where

$$\begin{aligned}
\mathbf{H}^{(q)} &= \boldsymbol{\Sigma}^{-1} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\mathbf{F} & \mathbf{1} \end{pmatrix}^{-1} \left[\boldsymbol{\Sigma} \bar{\mathbf{H}}^{(q)} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\mathbf{F} & \mathbf{1} \end{pmatrix} - \frac{\mathrm{d}}{\mathrm{d}\tau} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\mathbf{F} & \mathbf{1} \end{pmatrix} \right] \\
&= -\boldsymbol{\Sigma} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{F} & \mathbf{1} \end{pmatrix} \boldsymbol{\Sigma} \begin{pmatrix} \bar{\mathbf{H}}^{(q)}_{\bullet\bullet} & \bar{\mathbf{H}}^{(q)\bullet}_{\bullet} \\ \bar{\mathbf{H}}^{\bullet}_{(q)\bullet} & \bar{\mathbf{H}}^{\bullet\bullet}_{(q)} \end{pmatrix} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\mathbf{F} & \mathbf{1} \end{pmatrix} - \boldsymbol{\Sigma} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{F} & \mathbf{1} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{F} & \mathbf{0} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{1} & -\mathbf{F} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \begin{pmatrix} \bar{\mathbf{H}}^{(q)}_{\bullet\bullet} & \bar{\mathbf{H}}^{(q)\bullet}_{\bullet} \\ \bar{\mathbf{H}}^{\bullet}_{(q)\bullet} & \bar{\mathbf{H}}^{\bullet\bullet}_{(q)} \end{pmatrix} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\mathbf{F} & \mathbf{1} \end{pmatrix} - \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{F} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \quad .
\end{aligned} \tag{45}$$

The 3×3 submatrices of $\mathbf{H}^{(q)}$ are

$$\mathbf{H}^{(q)}_{\bullet\bullet} = \bar{\mathbf{H}}^{(q)}_{\bullet\bullet} - \bar{\mathbf{H}}^{(q)\bullet}_{\bullet}\mathbf{F} - \mathbf{F}\bar{\mathbf{H}}^{\bullet}_{(q)\bullet} + \mathbf{F}\bar{\mathbf{H}}^{\bullet\bullet}_{(q)}\mathbf{F} - \tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{F} \quad , \tag{46a}$$

$$\mathbf{H}^{(q)\bullet}_{\bullet} = \left(\mathbf{H}^{\bullet}_{(q)\bullet}\right)^{\mathrm{T}} = \bar{\mathbf{H}}^{(q)\bullet}_{\bullet} - \mathbf{F}\bar{\mathbf{H}}^{\bullet\bullet}_{(q)} \quad , \tag{46b}$$

$$\mathbf{H}^{\bullet\bullet}_{(q)} = \bar{\mathbf{H}}^{\bullet\bullet}_{(q)} \quad . \tag{46c}$$

Let us express the derivative of matrix (36), employing (11) and (43a,b),

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}F_{m3} = \tfrac{\mathrm{d}}{\mathrm{d}\tau}\left(h^{i}{}_{m}H^{(x)}_{i}\right) = H^{(x)}_{i}\tfrac{\mathrm{d}}{\mathrm{d}\tau}h^{i}{}_{m} + h^{i}{}_{m}H^{(x)}_{ik}H^{k}_{(x)} - h^{i}{}_{m}H^{(x)k}_{i}H^{(x)}_{k} = \bar{H}^{(q)}_{m3} - \bar{H}^{(q)k}_{m}H^{(q)}_{k} \quad . \tag{47}$$

Considering (36) and (44a,c), the 2×2 upper left submatrices of the 3×3 matrices (46a,b,c) are

$$H^{(q)}_{MN} = \bar{H}^{(q)}_{MN} - \bar{H}^{(q)3}_{M}H^{(q)}_{N} - H^{(q)}_{M}\bar{H}^{3}_{(q)N} + H^{(q)}_{M}\bar{H}^{33}_{(q)}H^{(q)}_{N} = \bar{H}^{(q)}_{MN} - (N{-}1)H^{(q)}_{M}H^{(q)}_{N} \quad , \tag{48a}$$

$$H^{(q)N}_{M} = \bar{H}^{(q)N}_{M} \quad , \tag{48b}$$

$$H^{MN}_{(q)} = \bar{H}^{MN}_{(q)} \quad . \tag{48c}$$

Considering (36), (43c), (44a,b,c), and (47), the other components of the 3×3 matrices (46a,b,c) are

$$H^{(q)}_{M3} = \bar{H}^{(q)}_{M3} - \bar{H}^{(q)k}_{M}H^{(q)}_{k} - H^{(q)}_{M}\bar{H}^{3}_{(q)3} + H^{(q)}_{M}\bar{H}^{3k}_{(q)}H^{(q)}_{k} + \bar{H}^{(q)k}_{M}H^{(q)}_{k} - \bar{H}^{(q)}_{M3} = 0 \quad , \tag{49a}$$

$$H^{(q)}_{33} = \bar{H}^{(q)}_{33} - \bar{H}^{(q)k}_{3}H^{(q)}_{k} - H^{(q)}_{k}\bar{H}^{k}_{(q)3} + H^{(q)}_{k}\bar{H}^{kl}_{(q)}H^{(q)}_{l} + \bar{H}^{(q)k}_{3}H^{(q)}_{k} - \bar{H}^{(q)}_{33} = 0 \quad , \tag{49b}$$

$$H^{(q)3}_{M} = \bar{H}^{(q)3}_{M} - H^{(q)}_{M}\bar{H}^{33}_{(q)} = 0 \quad , \tag{49c}$$

$$H^{(q)n}_{3} = \bar{H}^{(q)n}_{3} - H^{(q)}_{k}\bar{H}^{kn}_{(q)} = 0 \quad , \tag{49d}$$

$$H^{M3}_{(q)} = H^{3M}_{(q)} = 0 \quad , \tag{49e}$$

$$H^{33}_{(q)} = \bar{H}^{33}_{(q)} = N{-}1 \quad . \tag{49f}$$

Finally,

$$\mathbf{H}^{(q)} = \begin{pmatrix} H^{(q)}_{11} & H^{(q)}_{12} & 0 & H^{(q)1}_{1} & H^{(q)2}_{1} & 0 \\ H^{(q)}_{21} & H^{(q)}_{22} & 0 & H^{(q)1}_{2} & H^{(q)2}_{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ H^{1}_{(q)1} & H^{1}_{(q)2} & 0 & H^{11}_{(q)} & H^{12}_{(q)} & 0 \\ H^{2}_{(q)1} & H^{2}_{(q)2} & 0 & H^{21}_{(q)} & H^{22}_{(q)} & 0 \\ 0 & 0 & 0 & 0 & 0 & N{-}1 \end{pmatrix} \quad , \tag{50}$$

where

$$H^{(q)}_{MN} = h^{j}{}_{M}\left(H^{(x)}_{jk} - (N{-}1)H^{(x)}_{j}H^{(x)}_{k}\right)h^{k}{}_{N} \quad , \tag{51a}$$

$$H^{(q)N}_{M} = H^{N}_{(q)M} = h^{j}{}_{M}H^{(x)k}_{j}\hat{h}^{N}{}_{k} + h^{i}{}_{M}\tfrac{\mathrm{d}}{\mathrm{d}\tau}\hat{h}^{N}{}_{i} = h^{j}{}_{M}H^{(x)k}_{j}\hat{h}^{N}{}_{k} - \hat{h}^{N}{}_{i}\tfrac{\mathrm{d}}{\mathrm{d}\tau}h^{i}{}_{M} \quad , \tag{51b}$$

$$H^{MN}_{(q)} = \hat{h}^{M}{}_{j}H^{jk}_{(x)}\hat{h}^{N}{}_{k} \quad . \tag{51c}$$

9. Particular ray–centred coordinates

Basis vectors $h^i{}_M$ of the ray–centred coordinate system are tangent to the wavefront, in other respects they may be chosen arbitrarily. In numerical dynamic ray tracing in ray–centred coordinates, one has to select particular basis vectors along the whole ray, see e.g. Kendall *et al.* (1992). Here is one of the alternatives.

It follows from (51b) and from the orthogonality of $p_i^{(x)}$ and $h^i{}_M$, that the derivatives $H_M^{(q)\,N}$ in (50) would be zero if we chose

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau} h^i{}_M = \left(H^i_{(x)\,k} - (N{-}1) H^i_{(x)} H^{(x)}_k \right) h^k{}_M \quad , \tag{52a}$$

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau} \hat{h}^M{}_i = -\hat{h}^M{}_k \left(H^k_{(x)\,i} - H^{kj}_{(x)} H^{(x)}_j p^{(x)}_i \right) \quad . \tag{52b}$$

Equations (52a,b) guarantee relations (23) to be satisfied along the ray if they are satisfied at the initial point. If $H_M^{(q)\,N}$ in (50) are zero, the dynamic ray tracing system in ray–centred coordinates has a very similar form to that in isotropic media: $\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{Q}^{(q)}$ is a linear function of $\mathbf{P}^{(q)}$, and vice versa.

In isotropic media, equations (52a,b) yield the ray–centred coordinate system, the basis vectors of which do not rotate along the ray. Moreover, in isotropic media, the right–hand sides of (52a,b) are tangent to the ray, as in the ray–centred coordinates of Popov & Pšenčík (1978a).

10. Trivial dynamic ray tracing solutions

The linear dynamic ray tracing system (24) has six linearly independent solutions. There are two trivial linearly independent solutions of (24),

$$W^{\underline{m}}_{(q)\,3} = \begin{pmatrix} \delta^m{}_3 \\ 0_{m3} \end{pmatrix} \quad , \qquad W^{\underline{m}\,3}_{(q)} = \begin{pmatrix} (N{-}1)\tau\delta^m{}_3 \\ \delta_m{}^3 \end{pmatrix} \quad , \tag{53}$$

in covariant form [solutions of (41)], see (39b),

$$\bar{W}^{\underline{m}}_{(q)\,3} = \begin{pmatrix} \delta^m{}_3 \\ -H^{(q)}_m \end{pmatrix} \quad , \qquad \bar{W}^{\underline{m}\,3}_{(q)} = \begin{pmatrix} (N{-}1)\tau\delta^m{}_3 \\ -(N{-}1)\tau H^{(q)}_m + \delta_m{}^3 \end{pmatrix} \quad , \tag{54}$$

in Cartesian coordinates [solutions of (15)]), see (37b),

$$W^{\underline{m}}_{(x)\,3} = \begin{pmatrix} H^m_{(x)} \\ -H^{(x)}_m \end{pmatrix} = \tfrac{\mathrm{d}}{\mathrm{d}\tau} w^{\underline{m}}_{(x)} \;, \quad W^{\underline{m}\,3}_{(x)} = \begin{pmatrix} (N{-}1)\tau H^m_{(x)} \\ -(N{-}1)\tau H^{(x)}_m + p^{(x)}_m \end{pmatrix} = (N{-}1)\tau \tfrac{\mathrm{d}}{\mathrm{d}\tau} w^{\underline{m}}_{(x)} + \begin{pmatrix} 0^{m3} \\ p^{(x)}_m \end{pmatrix} \;. \tag{55}$$

11. Paraxial–ray propagator matrices

In Cartesian coordinates, the 6×6 paraxial–ray propagator matrix $\mathbf{\Pi}^{(x)}(\mathrm{B},\mathrm{A})$ from point A to point B is, Thomson & Chapman (1985),

$$\Pi^i_{(x)\,\underline{j}}(\mathrm{B},\mathrm{A}) = \frac{\partial w^i_{(x)}(\mathrm{B})}{\partial w^j_{(x)}(\mathrm{A})} \quad , \tag{56}$$

where the phase–space coordinates $w^i_{(x)}(\mathrm{A})$ at point A are considered to be the parameters of the 6–parametric system of rays, and $w^i_{(x)}(\mathrm{B})$ are the endpoints of ray elements of the fixed travel–time length $\tau(\mathrm{B},\mathrm{A})$. The individual columns of propagator matrix

$\mathbf{\Pi}^{(x)}(\mathrm{B},\mathrm{A})$ are the solutions of the dynamic ray tracing equations (15) with unit initial conditions at point A,

$$\mathbf{\Pi}^{(x)}(\mathrm{A},\mathrm{A}) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad . \tag{57}$$

Similarly, in ray–centred coordinates, the 6×6 paraxial–ray propagator matrix $\mathbf{\Pi}^{(q)}(\mathrm{B},\mathrm{A})$ from point A to point B is

$$\Pi^{\underline{m}}_{(q)\,\underline{n}}(\mathrm{B},\mathrm{A}) = \frac{\partial w^{\underline{m}}_{(q)}(\mathrm{B})}{\partial w^{\underline{n}}_{(q)}(\mathrm{A})} \quad . \tag{58}$$

Its structure is

$$\mathbf{\Pi}^{(q)}(\mathrm{B},\mathrm{A}) = \begin{pmatrix} \Pi^{1}_{(q)\,1}(\mathrm{B},\mathrm{A}) & \Pi^{1}_{(q)\,2}(\mathrm{B},\mathrm{A}) & 0 & \Pi^{11}_{(q)}(\mathrm{B},\mathrm{A}) & \Pi^{12}_{(q)}(\mathrm{B},\mathrm{A}) & 0 \\ \Pi^{2}_{(q)\,1}(\mathrm{B},\mathrm{A}) & \Pi^{2}_{(q)\,2}(\mathrm{B},\mathrm{A}) & 0 & \Pi^{21}_{(q)}(\mathrm{B},\mathrm{A}) & \Pi^{22}_{(q)}(\mathrm{B},\mathrm{A}) & 0 \\ 0 & 0 & 1 & 0 & 0 & (N{-}1)\tau(\mathrm{B},\mathrm{A}) \\ \Pi^{(q)}_{11}(\mathrm{B},\mathrm{A}) & \Pi^{(q)}_{12}(\mathrm{B},\mathrm{A}) & 0 & \Pi^{(q)\,1}_{1}(\mathrm{B},\mathrm{A}) & \Pi^{(q)\,2}_{1}(\mathrm{B},\mathrm{A}) & 0 \\ \Pi^{(q)}_{21}(\mathrm{B},\mathrm{A}) & \Pi^{(q)}_{22}(\mathrm{B},\mathrm{A}) & 0 & \Pi^{(q)\,1}_{2}(\mathrm{B},\mathrm{A}) & \Pi^{(q)\,2}_{2}(\mathrm{B},\mathrm{A}) & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} , \tag{59}$$

where the 4×4 propagator matrix $\Pi^{\underline{M}}_{(q)\,\underline{N}}(\mathrm{B},\mathrm{A})$ is the solution of the dynamic ray tracing equations

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\Pi^{\underline{M}}_{(q)\,\underline{N}} = \Sigma^{\underline{MJ}} H^{(q)}_{\underline{JK}} \Pi^{\underline{K}}_{(q)\,\underline{N}} \quad , \tag{60}$$

see (24), (50), and (53), with unit initial conditions at point A.

12. Numerical computation of paraxial–ray propagator matrices

In order to avoid unnecessary matrix multiplications, in an anisotropic medium it may be convenient to introduce the 6×6 matrix

$$W^{i}_{(x)\,\underline{n}}(\mathrm{B},\mathrm{A}) = \frac{\partial w^{i}_{(x)}(\mathrm{B})}{\partial w^{\underline{n}}_{(q)}(\mathrm{A})} \quad . \tag{61}$$

Four columns $W^{i}_{(x)\,\underline{N}}(\mathrm{B},\mathrm{A})$ of matrix (61) are the solutions of dynamic ray tracing equations (15) with initial conditions

$$W^{i}_{(x)\,\underline{N}}(\mathrm{A},\mathrm{A}) = h^{i}{}_{\underline{m}}(\mathrm{A}) \hat{F}^{\underline{m}}{}_{\underline{N}}(\mathrm{A}) \tag{62}$$

at point A, see (37b) and (39b). The two other columns $W^{i}_{(x)\underline{3}}(\mathrm{B},\mathrm{A})$ are

$$W^{m}_{(x)}{}_{3}(\mathrm{B},\mathrm{A}) = \frac{\mathrm{d}}{\mathrm{d}\tau} w^{m}_{(x)}(\mathrm{B}) \ , \quad W^{m3}_{(x)}(\mathrm{B},\mathrm{A}) = (N{-}1)\tau(\mathrm{B},\mathrm{A}) \frac{\mathrm{d}}{\mathrm{d}\tau} w^{m}_{(x)}(\mathrm{B}) + \begin{pmatrix} 0^{m3} \\ p^{(x)}_{m}(\mathrm{B}) \end{pmatrix} , \tag{63}$$

see (55). Then, see (37b) and (39b),

$$\Pi^{i}_{(x)\,\underline{j}}(\mathrm{B},\mathrm{A}) = W^{i}_{(x)\,\underline{n}}(\mathrm{B},\mathrm{A}) F^{\underline{n}}{}_{\underline{k}}(\mathrm{A}) \hat{h}^{\underline{k}}{}_{\underline{j}}(\mathrm{A}) \quad , \tag{64}$$

and

$$\Pi^{\underline{m}}_{(q)\,\underline{n}}(\mathrm{B},\mathrm{A}) = F^{\underline{m}}{}_{\underline{k}}(\mathrm{B}) \hat{h}^{\underline{k}}{}_{\underline{i}}(\mathrm{B}) W^{i}_{(x)\,\underline{n}}(\mathrm{B},\mathrm{A}) \quad . \tag{65}$$

Transformation matrices $\hat{h}^{\underline{m}}{}_{i}$ and $F^{\underline{m}}{}_{\underline{n}}$ are defined by (32) and (35).

Appendix A: Cartesian coordinates

Let us denote by ξ^i those coordinates with respect to which coefficients c^{ijkl} of the elastodynamic equation

$$\frac{\partial}{\partial \xi^i}\left(c^{ijkl}\frac{\partial}{\partial \xi^l}u_k\right) = \rho\frac{\partial^2}{\partial t^2}u_j \qquad (\mathrm{A}-1)$$

are measured. Note that these coordinates may be local, they need not form a global coordinate system, especially if they differ from the model coordinates introduced in Appendix B. By *Cartesian metric* we shall understand a metric such that its metric tensor in the ξ^i–coordinates is an identity matrix. We shall call *Cartesian coordinates* any coordinates x^i in which the Cartesian metric tensor is constant, and *orthonormal Cartesian coordinates* any coordinates x^i in which the Cartesian metric tensor is an identity matrix.

As a rule, the coefficients of the elastodynamic equation are measured with respect to an ordinary Euclidean coordinate system using such length units as kilometres or feet, although they are often considered to be the functions of geographic coordinates expressed in degrees. In this case, the Cartesian coordinates are the same as the ordinary Euclidean coordinates used in all branches of physics. On the other hand, if the coefficients were expressed in terms of geographic spherical coordinate system units (e.g. propagation velocity in degrees per second), the Cartesian coordinates would be represented by geographic spherical coordinates.

Appendix B: Model coordinates

Model coordinates μ^i are coordinates such that the coefficients of the elastodynamic equation are given functions of μ^i. For instance, if the elastodynamic coefficients are functions of geographic longitude, latitude, and the distance from the centre of the Earth, the model coordinates μ^i are these three geographic spherical coordinates. Model coordinates μ^i need not coincide with Cartesian coordinates: for instance, if the model coordinates μ^i are geographic spherical coordinates while the elastodynamic coefficients are measured in the SI units (e.g. velocity in km/s).

If model coordinates μ^i do not coincide with Cartesian coordinates x^i and we wish to perform numerical computations in *Cartesian coordinates*, functions

$$\mu^k = \mu^k(x^i) \quad , \quad \frac{\partial \mu^k}{\partial x^m} = \frac{\partial \mu^k}{\partial x^m}(x^i) \quad , \quad \frac{\partial^2 \mu^k}{\partial x^m \partial x^n} = \frac{\partial^2 \mu^k}{\partial x^m \partial x^n}(x^i) \quad , \quad \dots \qquad (\mathrm{B}-1)$$

should be known. In this case, all equations may be expressed in Cartesian coordinates x^i, and the derivatives with respect to model coordinates μ^i may be transformed to Cartesian coordinates x^i during numerical computations by means of a special routine.

If model coordinates μ^i do not coincide with Cartesian coordinates x^i and we wish to perform numerical computations in *model coordinates* μ^i (see, e.g., Červený, Klimeš & Pšenčík 1988), at least the Cartesian metric tensor

$$\frac{\partial \xi^m}{\partial \mu^i}\frac{\partial \xi^m}{\partial \mu^j} = g_{ij}(\mu^l) \qquad (\mathrm{B}-2)$$

and the corresponding Christoffel symbols

$$\frac{\partial^2 \xi^m}{\partial \mu^i \partial \mu^j}\frac{\partial \mu^k}{\partial \xi^m} = \Gamma_{ij}^{\,k}(\mu^l) \qquad (\mathrm{B}-3)$$

should be known if the equations contain derivatives of elastodynamic coefficients up to the second order. In this case, all equations should be expressed in model coordinates μ^i.

The transformation of equations from Cartesian coordinates x^i to model coordinates μ^i is extremely simple: all partial derivatives with respect to Cartesian coordinates x^i are replaced by covariant derivatives with respect to model coordinates μ^i. Here the word "covariant" is related to the Cartesian metric.

Thus, the theory as a whole may be developed in Cartesian coordinates x^i, assuming the model coordinates to coincide with them,

$$\mu^i = x^i \quad , \tag{B - 4}$$

and the final equations can, if required, be transformed to non–Cartesian model coordinates μ^i.

Acknowledgements

The author is indebted to Professor Vlastislav Červený for many invaluable discussions on the topic of this paper, and to Dr. Ivan Pšenčík for his helpful suggestions and comments regarding the manuscript.

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