Ray propagator matrices in 3-D anisotropic inhomogeneous layered media

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Summary

Ray propagator matrices contain the complete solutions to the system of dynamic ray tracing equations connected with a given reference ray. They play an important role in studying the properties of complete four-parameteric systems of paraxial rays and offer many applications in both numerical modeling and practical interpretational problems of seismic ray fields in the high-frequency asymptotic approximation.

Traditionally, ray propagator matrices have been expressed either in Cartesian coordinates or in ray-centered coordinates, connected with a reference ray. Both coordinate systems have certain advantages. For ray-centered coordinates, the dimensions of ray propagator matrices can be easily reduced from 6×6 to 4×4 (in a 3-D medium), thereby reflecting the strictly four-parameteric nature of a general paraxial ray field. On the other hand, in Cartesian coordinates, the computations are conceptually simpler and generally valid in isotropic and anisotropic media. In a Cartesian coordinate system, the dynamic ray tracing system and ray propagator matrices are well-known both for isotropic and anisotropic layered media. In ray-centered coordinates, the dynamic ray tracing system and ray propagator matrices are known for isotropic layered structures and for anisotropic smooth media, but not for anisotropic media with structural interfaces.

We propose a simple and invertible transformation between ray-propagator matrices in both coordinate systems. It allows to perform conventional dynamic ray tracing in Cartesian coordinates, and to transform the resulting ray-propagator matrix to ray-centered coordinates at any point of the ray where we need it. This avoids dynamic ray tracing in ray-centered coordinates altogether. Vice versa, we can compute, at any point of the reference ray, the ray propagator matrix in Cartesian coordinates by dynamic ray tracing in ray-centered coordinates. We propose several alternative versions of the transformation, each of them equally valid in isotropic and anisotropic media.

Seismic Waves in Complex 3-D Structures, Report 16 (Department of Geophysics, Charles University, Praha 2006), pp. 87–114.

For rays hitting a structural interfaces, the ray propagator matrix has to be transformed across the interface. The relevant transformation matrix is usually referred to as the interface propagator matrix. In Cartesian coordinates, the 6×6 interface propagator matrix has been published before, but in ray-centered coordinates only for the case of isotropic media. Based on the transformation from Cartesian to ray-centered coordinates, we present the 6×6 and 4×4 interface propagator matrices in ray-centered coordinates, valid for general isotropic and anisotropic media. The 4×4 interface propagator matrix in ray-centered coordinates can be factorized and used to derive the 4×4 surface-to-surface paraxial matrices. These matrices allow to relate the paraxial ray properties at different surfaces crossed by the reference ray and offer many important applications.

Keywords: Seismic ray theory, seismic anisotropy, lateral heterogeneities, layered media.

1 Introduction

Dynamic ray tracing (abbreviated DRT and also called paraxial ray tracing) consists of solving a system of several linear ordinary differential equations of the first order along a reference ray. It has found useful applications in the investigation of an orthonomic (two-parameteric) system of rays connected with the reference ray. It can be used to determine geometrical spreading (needed in the computation of amplitudes), wavefront curvatures, etc., of the elementary wave propagating along the ray. It can also be used to compute the relevant propagator matrix. The propagator matrix corresponding to the dynamic ray tracing system is usually referred to as the dynamic ray tracing propagator matrix, or briefly the ray propagator matrix. Here we refer to it as the ray propagator matrix. The ray propagator matrix is very convenient in studying the complete (four-parameteric) system of paraxial rays connected with the reference ray under consideration.

The dynamic ray tracing system and relevant propagator matrices play a very important role in the paraxial ray methods, in which the kinematic quantities are studied in the so-called paraxial vicinity of the reference ray. We speak of paraxial rays, paraxial travel times, and paraxial slowness vector. They can be used to compute the second-order and higher-order spatial derivatives of travel times, to investigate chaotic rays and evaluate Lyapunov exponents, and to study the reciprocity relations along the ray. Finally, the ray propagator matrix is essential in various extensions of the ray method, such as the method of Gaussian beams and Gaussian packets, the Maslov-Chapman method, the Kirchhoff-Helmholtz method, ray perturbation theories, etc. For more details on paraxial ray methods see Červený (2001, Chap. 4), and Moser and Červený (2006), where other references are given. See also Section 8. For various approaches to kinematic and dynamic ray tracing in inhomogeneous anisotropic media we refer the reader to Červený (1972, 2001), Hanyga (1982), Gajewski and Pšenčík (1987, 1990), Norris (1987), Shearer and Chapman (1989), Farra (1989), Kendall, Guest and Thomson (1992), Klimeš (1994, 2006), Farra and LeBégat (1995), Bakker (1996), Hanyga et al. (2001), Gjoystdal et al. (2002), Iversen (2004a), Moser (2004), and Chapman (2004), where many other references can be found. In several of these references, ray propagator matrices are also discussed.

The dynamic ray tracing system and ray propagator matrices are commonly expressed in the global Cartesian coordinate system, or in the ray-centered coordinate system, connected to a suitable reference ray. For isotropic media, the ray-centered coordinate system was first introduced to seismology by Popov and Pšenčík (1978a,b), see also Červený, Klimeš and Pšenčík (1988). For anisotropic media, see Klimeš (1994, 2006). In global Cartesian coordinates, the ray propagator matrices are 6×6, whereas for ray-centered coordinates they are 6×6 or 4×4 - corresponding to systems of six or four differential equations, respectively. The propagators in both coordinate systems satisfy the important symplectic and chain properties. At intersections of the reference ray with structural interfaces, ray propagator matrices must be chained and the so-called interface propagator matrix must be included in the chain. The problem of the transformation of the dynamic ray tracing system across the structural interface has been solved by various approaches. For isotropic media, see Červený, Langer and Pšenčík (1974) in Cartesian coordinates, Popov and Pšenčík (1978a,b) and Červený and Hron (1980) in ray-centered coordinates. For anisotropic media, see Gajewski and Pšenčík (1990), and Farra and LeBégat (1995) in Cartesian coordinates. Farra and LeBégat (1995) showed that some previously derived transformation equations do not satisfy the symplecticity relation. In Cartesian coordinates, a suitable form of the interface propagator matrix satisfying symplecticity was proposed by Moser (2004), and for some other coordinate systems by Červený (2001) (e.g., for the wavefront orthonormal coordinate system). For ray-centered coordinates and anisotropic media, however, the derivation of the interface propagator matrix has not yet been reported in the seismological literature.

Let us briefly discuss the advantages and disadvantages of ray propagator matrices in global Cartesian and ray-centered coordinate systems. The main advantage of 6×6 ray propagator matrices in Cartesian coordinates is that the dynamic ray tracing system has a general and simple structure, and that the interface transformation matrix is well known. However, from the six linearly independent solutions two are redundant: the so-called ray-tangent and non-eikonal solutions. These redundant solutions complicate the solution of various boundary-value problems of the general system of rays, which is strictly four-parameteric. Contrary to the 6×6 propagator matrix in Cartesian coordinates, the redundant solutions can be immediately removed from the 6×6 propagator matrix in ray-centered coordinates, and a reduction to 4×4 form is straightforward. For anisotropic media, however, the dynamic ray tracing system in ray-centered coordinates is more complicated than in Cartesian coordinates. Among these complications is the requirement to solve an additional differential equation along the ray to determine the basis vectors of the ray-centered coordinate system (see Klimeš, 1994, 2006; Červený, 2001).

In this paper, we show that the 4×4 ray propagator matrix in ray-centered coordinates can be computed by dynamic ray tracing in Cartesian coordinates. Dynamic ray tracing in ray-centered coordinates is not required at all. Moreover, the differential equation for the basis vectors of the ray-centered coordinate system along the ray need not be solved. Two basic approaches are proposed. In the first approach, the ray propagator matrix in ray-centered coordinates is obtained by some transformation of the ray propagator matrix in Cartesian coordinates at the initial and end points of the ray. If needed, the ray propagator matrix in ray-centered coordinates can also be computed in the same way at any intermediate point of the ray. In the second approach, the ray propagator matrix in ray-centered coordinates is obtained from four solutions of the dynamic ray tracing system in Cartesian coordinates, with strictly specified initial conditions. Thus, only four solutions are needed in this approach, not six as in the previous case. Both approaches are invertible and can also be used to compute the 6×6 ray propagator matrix in Cartesian coordinates from the 6×6 (or 4×4) ray propagator matrix in ray-centered coordinates.

The proposed transformations between ray propagator matrices in Cartesian and ray-centered coordinate systems are also used to derive the 6×6 and 4×4 interface propagator matrices in ray-centered coordinates from the known interface propagator matrices in Cartesian coordinates. The interface propagator matrices can be factorized and used to derive the 4×4 surface-to-surface paraxial matrices in ray-centered coordinates, which relate the paraxial ray quantities at different surfaces crossed by the reference ray. The surfaces may represent structural interfaces, the surface of the Earth, isochrone surfaces, or formal surfaces. Actually, the formal surfaces may be introduced at any point of the reference ray where needed. We require that the surfaces representing the structural interfaces do not intersect in the paraxial vicinity of the reference ray.

Briefly to the content of the paper. The kinematic and dynamic ray tracing and ray propagator matrices in Cartesian coordinates are reviewed in Section 2. Section 3 introduces the ray-centered coordinate system and its basis vectors (both contravariant and covariant), gives the dynamic ray tracing system in ray-centered coordinates and the expression for the ray propagator matrix in ray-centered coordinates. Section 4 specifies the general transformation relation between the ray propagator matrices corresponding to two coordinate systems, derived in Červený (2001, eq. (4.3.38)), to Cartesian and ray-centered coordinate systems. Basic relations (61) with (59) are derived. The transformations are fully invertible; they can be used in both directions. In Section 5, we discuss an alternative equation (64) for the ray propagator matrix in ray-centered coordinates, which requires the determination of only four solutions of the dynamic ray tracing equation in Cartesian coordinates. In Section 6, simple expressions for the 4×4 and 6×6 interface propagator matrices in ray-centered coordinates are derived. In Section 7, it is shown that both the 6×6 and 4×4 interface propagator matrices in ray-centered coordinates may be factorized and used to derive the surface-to-surface paraxial matrices in ray-centered coordinates. Finally, Section 8 offers some concluding remarks.

The notations in the paper are as follows: 3×3 and 6×6 matrices and 3×1 vectors are denoted by Roman boldface symbols, 2×2 and 4×4 matrices and 2×1 vectors by Italic boldface symbols. The symbol T in the superscript of a matrix means "transpose", and the symbol -T in the superscript denotes "inverse transpose". The lowercase indices i, j, k, ... take the values 1, 2, 3, and the uppercase indices $I, J, K, ...$ the values 1, 2. The Einstein summation convention is applied to repeated indices in the same product.

2 Dynamic ray tracing and ray-propagator matrices in Cartesian coordinates

Consider the eikonal equation for travel-time field $T(\mathbf{x})$ in Hamiltonian form

$$\mathcal{H}(\mathbf{x}, \mathbf{p}) = 0 \ , \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian, $\mathbf{x}$ is the position vector, and $\mathbf{p}$ the slowness vector, $\mathbf{p} = \partial T/\partial \mathbf{x}$. We consider the Hamiltonians which are homogeneous functions of the second degree in $\mathbf{p}$ (with a possible additional constant). The kinematic ray tracing equations then read

$$\mathrm{d}\mathbf{x}/\mathrm{d}\tau = \boldsymbol{\mathcal{U}} = \partial\mathcal{H}/\partial\mathbf{p} \ , \quad \mathrm{d}\mathbf{p}/\mathrm{d}\tau = \boldsymbol{\eta} = -\partial\mathcal{H}/\partial\mathbf{x} \ . \tag{2}$$

Here τ is a monotonically increasing sampling parameter along the ray, which represents the travel time. The initial point of the ray corresponds to $\tau = \tau_0$. Equations (2) also define the ray velocity vector $\boldsymbol{\mathcal{U}}$ (also called the group velocity vector) and vector $\boldsymbol{\eta}$, which will be broadly used in this paper.

The dynamic ray tracing system is designed to compute two 3×1 matrices $\mathbf{Q}^{(x)} \equiv (Q_1^{(x)}, Q_2^{(x)}, Q_3^{(x)})^T$ and $\mathbf{P}^{(x)} \equiv (P_1^{(x)}, P_2^{(x)}, P_3^{(x)})^T$ along the ray,

$$\mathbf{Q}^{(x)} = \partial\mathbf{x}/\partial\gamma \ , \quad \mathbf{P}^{(x)} = \partial\mathbf{p}/\partial\gamma \ , \tag{3}$$

where γ is an arbitrary ray parameter, or any of the initial values $x_{i0} = x_i(\tau_0)$, $p_{i0} = p_i(\tau_0)$. Taking the partial derivative of (2) with respect to γ, we obtain the dynamic ray tracing system in Cartesian coordinates

$$\begin{aligned} \mathrm{d}\mathbf{Q}^{(x)}/\mathrm{d}\tau &= \mathbf{A}^{(x)}\mathbf{Q}^{(x)} + \mathbf{B}^{(x)}\mathbf{P}^{(x)} \ , \\ \mathrm{d}\mathbf{P}^{(x)}/\mathrm{d}\tau &= -\mathbf{C}^{(x)}\mathbf{Q}^{(x)} - \mathbf{D}^{(x)}\mathbf{P}^{(x)} \ . \end{aligned} \tag{4}$$

Here $\mathbf{A}^{(x)}$, $\mathbf{B}^{(x)}$, $\mathbf{C}^{(x)}$ and $\mathbf{D}^{(x)}$ are 3×3 matrices, given by relations

$$\begin{aligned} \mathbf{A}^{(x)} = \partial^2\mathcal{H}/\partial\mathbf{p}\partial\mathbf{x} \ , \quad \mathbf{B}^{(x)} = \partial^2\mathcal{H}/\partial\mathbf{p}\partial\mathbf{p} \ , \\ \mathbf{C}^{(x)} = \partial^2\mathcal{H}/\partial\mathbf{x}\partial\mathbf{x} \ , \quad \mathbf{D}^{(x)} = \partial^2\mathcal{H}/\partial\mathbf{x}\partial\mathbf{p} \ . \end{aligned} \tag{5}$$

The solutions of the dynamic ray tracing equation must satisfy the constraint relation

$$\boldsymbol{\mathcal{U}}^T\mathbf{P}^{(x)} - \boldsymbol{\eta}^T\mathbf{Q}^{(x)} = 0 \ , \tag{6}$$

which follows from (1). The superscript (x) in Equations (3)-(6), and in the following, indicates that the quantities are expressed in Cartesian coordinates.

Dynamic ray tracing system (4) consists of six linear ordinary differential equations of the first order for $Q_i^{(x)}$ and $P_i^{(x)}$, and has six linearly independent solutions. Consequently, we can construct the 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$, which is defined as the fundamental matrix of (4), subject to initial conditions $\mathbf{\Pi}^{(x)}(\tau_0, \tau_0) = \mathbf{I}$, where $\mathbf{I}$ is the 6×6 identity matrix. Propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ has a number of useful properties. The most important of them is symplecticity:

$$\mathbf{\Pi}^{(x)T}\mathbf{J}\mathbf{\Pi}^{(x)} = \mathbf{J} \ , \tag{7}$$

where $\mathbf{J}$ is a 6×6 matrix given by the formula

$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix} . \tag{8}$$

Here $\mathbf{0}$ is a 3×3 zero matrix, and $\mathbf{I}$ the 3×3 identity matrix. The continuation property of $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ reads

$$\begin{pmatrix} \mathbf{Q}^{(x)}(\tau) \\ \mathbf{P}^{(x)}(\tau) \end{pmatrix} = \mathbf{\Pi}^{(x)}(\tau, \tau_0) \begin{pmatrix} \mathbf{Q}^{(x)}(\tau_0) \\ \mathbf{P}^{(x)}(\tau_0) \end{pmatrix} . \tag{9}$$

Equation (9) can also be expressed in the form

$$\begin{pmatrix} \delta\mathbf{x}(\tau) \\ \delta\mathbf{p}(\tau) \end{pmatrix} = \mathbf{\Pi}^{(x)}(\tau, \tau_0) \begin{pmatrix} \delta\mathbf{x}(\tau_0) \\ \delta\mathbf{p}(\tau_0) \end{pmatrix} , \tag{10}$$

where $\delta\mathbf{x}$ and $\delta\mathbf{p}$ are small perturbations of $\mathbf{x}$ and $\mathbf{p}$ around the reference ray. Equation (10) shows well the physical meaning of ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates. The chain rule states that

$$\mathbf{\Pi}^{(x)}(\tau, \tau_0) = \mathbf{\Pi}^{(x)}(\tau, \tau_1)\mathbf{\Pi}^{(x)}(\tau_1, \tau_0) , \tag{11}$$

for any τ_1 situated on the ray, and Liouville's theorem yields $\det(\mathbf{\Pi}^{(x)}(\tau, \tau_0)) = 1$ for any τ. Finally, the symplectic property yields a simple relation for the inverse of $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$,

$$\begin{pmatrix} \mathbf{\Pi}_{11} & \mathbf{\Pi}_{12} \\ \mathbf{\Pi}_{21} & \mathbf{\Pi}_{22} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{\Pi}_{22}^T & -\mathbf{\Pi}_{12}^T \\ -\mathbf{\Pi}_{21}^T & \mathbf{\Pi}_{11}^T \end{pmatrix} , \tag{12}$$

where $\mathbf{\Pi}_{11}, \mathbf{\Pi}_{12}, \mathbf{\Pi}_{21}$ and $\mathbf{\Pi}_{22}$ are 3×3 submatrices of $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$. Note that the partial derivatives with respect to γ in $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ are taken for a fixed travel time $T = \tau$.

As the complete system of rays is four-parameteric, two solutions in $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ are redundant. The expressions for these two solutions can be found explicitly. The first of them is the so-called ray-tangent solution:

$$\mathbf{Q}^{(x)} = \boldsymbol{\mathcal{U}} , \qquad \mathbf{P}^{(x)} = \boldsymbol{\eta} , \tag{13}$$

and the latter is the non-eikonal solution,

$$\mathbf{Q}^{(x)} = (\tau - \tau_0)\boldsymbol{\mathcal{U}} , \quad \mathbf{P}^{(x)} = \mathbf{p} + (\tau - \tau_0)\boldsymbol{\eta} . \tag{14}$$

For more details on dynamic ray tracing and ray propagator matrices in Cartesian coordinates in inhomogeneous anisotropic media and on the ray-tangent and non-eikonal solutions see Červený (2001), and Chapman (2004), where many other references are given. Chapman (2004, p.152) also presents a physical explanation of the non-eikonal solution, given by R. Burridge.

The above theory would not be complete without considering structural interfaces in the model. Ray-tracing equations (2), dynamic ray tracing equations (4) and the expressions for the ray propagator matrix should be modified when the ray crosses a structural interface. Under "crossing the interface" we understand not only transmission, but also reflection. We consider a structural interface Σ, which separates two parts of the medium with different smooth distributions of the elastic moduli and density. We use the parameteric description of the interface, given by relation $\mathbf{x} = \mathbf{g}(u_1, u_2)$, where u_I, $I = 1, 2$, are the Gaussian coordinates of the surface. As a special case of u_1, u_2, we can also consider local Cartesian coordinates in a plane tangent to interface Σ at the reference ray Ω. At any point of Σ, the interface can be approximated to the second order in u_I by the relation

$$\mathbf{x}(u_I) = \mathbf{x}_0 + \mathbf{g}_I u_I + \tfrac{1}{2}\mathbf{g}_{IJ} u_I u_J \ . \tag{15}$$

Here $\mathbf{g}_I = \partial \mathbf{g}/\partial u_I$ are vectors tangent to Σ at $\mathbf{x} = \mathbf{x}_0$, and $\mathbf{g}_{IJ} = \partial^2 \mathbf{g}/\partial u_I \partial u_J$ are related to the curvature matrix of the interface at $\mathbf{x} = \mathbf{x}_0$, $I, J = 1, 2$. See more details in Moser and Červený (2006).

Let us consider a ray incident at interface Σ at $\mathbf{x}_0$, and denote the relevant sampling parameter τ at the point of incidence τ_Σ. At τ_Σ, vectors $\mathbf{p}$, $\boldsymbol{\mathcal{U}}$ and $\boldsymbol{\eta}$ are known from kinematic ray tracing (2). Using Snell's law, we can compute these quantities also at the reflection/transmission point of the selected reflected/transmitted wave. We denote them with a tilde, namely $\tilde{\tau}_\Sigma$, $\tilde{\mathbf{p}}$, $\tilde{\boldsymbol{\mathcal{U}}}$, $\tilde{\boldsymbol{\eta}}$. Although the points of incidence τ_Σ and of reflection/transmission $\tilde{\tau}_\Sigma$ coincide, we shall consider them formally as two different points.

The matrices $\tilde{\mathbf{Q}}^{(x)}$, $\tilde{\mathbf{P}}^{(x)}$ at the reflection/transmission point $\tilde{\tau}_\Sigma$, and $\mathbf{Q}^{(x)}$, $\mathbf{P}^{(x)}$ at the point of incidence τ_Σ are then related by the equation,

$$\begin{bmatrix} \tilde{\mathbf{Q}}^{(x)} \\ \tilde{\mathbf{P}}^{(x)} \end{bmatrix} = \boldsymbol{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma) \begin{bmatrix} \mathbf{Q}^{(x)} \\ \mathbf{P}^{(x)} \end{bmatrix} , \tag{16}$$

where $\boldsymbol{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ is the so-called interface propagator matrix in Cartesian coordinates. A particularly concise form of the 6×6 interface propagator matrix was given by Moser (2004),

$$\boldsymbol{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma) = \begin{bmatrix} \tilde{\mathbf{X}}\mathbf{X}^{-1} & \mathbf{0} \\ \tilde{\mathbf{X}}^{-T}\mathbf{R}\mathbf{X}^{-1} & \tilde{\mathbf{X}}^{-T}\mathbf{X}^T \end{bmatrix} , \tag{17}$$

where 3×3 matrices $\mathbf{X}$ and $\tilde{\mathbf{X}}$ are given by relations

$$\mathbf{X} = (\mathbf{g}_1, \mathbf{g}_2, \boldsymbol{\mathcal{U}}) \ , \quad \tilde{\mathbf{X}} = (\mathbf{g}_1, \mathbf{g}_2, \tilde{\boldsymbol{\mathcal{U}}}) \ , \tag{18}$$

and the 3×3 matrix $\mathbf{R}$ reads

$$\mathbf{R} = \begin{bmatrix} \mathbf{g}_{IJ}^T(\tilde{\mathbf{p}} - \mathbf{p}) & \mathbf{g}_I^T(\tilde{\boldsymbol{\eta}} - \boldsymbol{\eta}) \\ \mathbf{g}_J^T(\tilde{\boldsymbol{\eta}} - \boldsymbol{\eta}) & \tilde{\boldsymbol{\eta}}^T\tilde{\boldsymbol{\mathcal{U}}} - \boldsymbol{\eta}^T\boldsymbol{\mathcal{U}} \end{bmatrix} . \tag{19}$$

The interface propagator matrix $\boldsymbol{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ is symplectic, satisfies the relation $\det \boldsymbol{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma) = 1$ and preserves constraint relation (6) across the interface.

For the following sections, it will be useful to express the matrix inversions in (17) explicitly. We introduce 3×3 matrices

$$\mathbf{U} = \mathbf{X}^{-T} = (\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3) \ , \quad \tilde{\mathbf{U}} = \tilde{\mathbf{X}}^{-T} = (\tilde{\mathbf{h}}_1, \tilde{\mathbf{h}}_2, \tilde{\mathbf{h}}_3) \ . \tag{20}$$

Here $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3$ can be calculated from $\mathbf{g}_1, \mathbf{g}_2, \boldsymbol{\mathcal{U}}$ by relations,

$$\mathbf{h}_1 = \frac{\mathbf{g}_2 \times \boldsymbol{\mathcal{U}}}{\boldsymbol{\mathcal{U}}^T(\mathbf{g}_1 \times \mathbf{g}_2)} \ , \quad \mathbf{h}_2 = \frac{\boldsymbol{\mathcal{U}} \times \mathbf{g}_1}{\boldsymbol{\mathcal{U}}^T(\mathbf{g}_1 \times \mathbf{g}_2)} \ , \quad \mathbf{h}_3 = \frac{\mathbf{n}^\Sigma}{\boldsymbol{\mathcal{U}}^T\mathbf{n}^\Sigma} \ , \tag{21}$$

where $\mathbf{n}^\Sigma$ is a vector normal to Σ at a point of incidence (not necessarily unit). Similarly, $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ can be calculated from $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3$ as follows:

$$\mathbf{g}_1 = \frac{\mathbf{h}_2 \times \mathbf{h}_3}{\mathbf{h}_3^T(\mathbf{h}_1 \times \mathbf{h}_2)} \ , \quad \mathbf{g}_2 = \frac{\mathbf{h}_3 \times \mathbf{h}_1}{\mathbf{h}_3^T(\mathbf{h}_1 \times \mathbf{h}_2)} \ , \quad \mathbf{g}_3 = \boldsymbol{\mathcal{U}} \ . \tag{22}$$

Similar expressions are obtained also for the tilded vectors; we only need to take into account that $\tilde{\mathbf{g}}_1 = \mathbf{g}_1, \tilde{\mathbf{g}}_2 = \mathbf{g}_2$. The expression for the 6×6 interface propagator matrix $\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ in Cartesian coordinates then reads

$$\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma) = \begin{pmatrix} \tilde{\mathbf{X}}\mathbf{U}^T & \mathbf{0} \\ \tilde{\mathbf{U}}\mathbf{R}\mathbf{U}^T & \tilde{\mathbf{U}}\mathbf{X}^T \end{pmatrix} \ , \tag{23}$$

see (17) and (20).

Note that vectors $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3 = \boldsymbol{\mathcal{U}}$ represent the contravariant basis vectors, and $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3 = \mathbf{n}^\Sigma/\boldsymbol{\mathcal{U}}^T\mathbf{n}^\Sigma$ the covariant basis vector in the local nonorthogonal coordinate system $u_1, u_2, u_3 = \tau$ at the point of incidence. At the point of reflection/transmission, the contravariant basis vectors are $\tilde{\mathbf{g}}_1 = \mathbf{g}_1$, $\tilde{\mathbf{g}}_2 = \mathbf{g}_2, \tilde{\mathbf{g}}_3 = \tilde{\boldsymbol{\mathcal{U}}}$, and covariant $\tilde{\mathbf{h}}_1, \tilde{\mathbf{h}}_2$, $\tilde{\mathbf{h}}_3 = \mathbf{n}^\Sigma/\tilde{\boldsymbol{\mathcal{U}}}^T\mathbf{n}^\Sigma$. Basis vectors satisfy the relations

$$\mathbf{h}_k^T\mathbf{g}_l = \delta_{kl} \ , \quad \tilde{\mathbf{h}}_k^T\tilde{\mathbf{g}}_l = \delta_{kl} \ , \quad \mathbf{h}_k\mathbf{g}_k^T = \mathbf{I} \ , \quad \tilde{\mathbf{h}}_k\tilde{\mathbf{g}}_k^T = \mathbf{I} \ , \tag{24}$$

where $\mathbf{I}$ is the 3×3 identity matrix. Vectors $\mathbf{g}_1$ and $\mathbf{g}_2$ are tangent to surface Σ, $\mathbf{h}_1, \mathbf{h}_2$ and $\tilde{\mathbf{h}}_1, \tilde{\mathbf{h}}_2$ are perpendicular to the ray. Vectors $\mathbf{g}_1$ and $\mathbf{g}_2$ need not be unit and mutually perpendicular, and similarly $\mathbf{h}_1$ and $\mathbf{h}_2$ and $\tilde{\mathbf{h}}_1$ and $\tilde{\mathbf{h}}_2$.

In a layered medium with structural interfaces, the ray propagator matrix can be chained and the interface propagator matrix should be included in the chain at any point of incidence. For example, if the ray crosses one interface at τ_Σ between τ_0 and τ, we obtain

$$\mathbf{\Pi}^{(x)}(\tau, \tau_0) = \mathbf{\Pi}^{(x)}(\tau, \tilde{\tau}_\Sigma)\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma)\mathbf{\Pi}^{(x)}(\tau_\Sigma, \tau_0) \ . \tag{25}$$

For a more thorough treatment see Moser (2004), where a general sampling parameter τ along the ray is used (not necessarily the travel time).

A terminological note. The term *interface propagator matrix* was used by Červený (2001) and Moser (2004), to emphasize the fact that the matrix transforms the ray propagator matrix across the interface. Analogous term *wave propagator for the interface* was also used by Kennett (1983, p. 111) in the stress-displacement propagator formalism for 1-D layered media.

3 Ray-centered coordinate systems

The ray-centered coordinate system $\mathbf{q} = (q_1, q_2, q_3)$ connected with the reference ray Ω in an inhomogeneous anisotropic medium can be introduced in many alternative ways. For an up-to-date review of various posibilities see Klimeš (2006). One of the simplest options is introduced by the relation, see Klimeš (1994, 2006):

$$x_i(q_j) = x_{i0}(q_3) + H_{iM}(q_3)q_M \ , \tag{26}$$

$i = 1, 2, 3$, and $M = 1, 2$. The reference ray Ω is specified by the relation $x_i(q_3) = x_{i0}(q_3)$ and represents the q_3-coordinate line of the nonorthogonal ray-centered coordinate system, and $q_3 = \tau$, the travel-time along the ray. Coordinates q_1 and q_2 uniquely specify the position of a point in the plane tangent to the wavefront intersecting the reference ray Ω for a fixed q_3. For $q_1 = q_2 = 0$, the point is situated directly on the reference ray Ω.

We introduce the 3×3 transformation matrix $\mathbf{H}$ from Cartesian coordinates x_i to ray-centered coordinates q_m,

$$H_{im} = \partial x_i / \partial q_m \ , \tag{27}$$

$i, m = 1, 2, 3$. The contravariant basis vectors of the ray-centered coordinate system $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are given by the relations

$$\mathbf{H} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 = \boldsymbol{\mathcal{U}}) \ . \tag{28}$$

$\mathbf{e}_1$ and $\mathbf{e}_2$ are situated in the wavefront tangent plane, $\mathbf{e}_3$ coincides with the ray velocity vector $\boldsymbol{\mathcal{U}}$, tangent to the ray.

Covariant basis vectors $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ are given by the relation

$$\mathbf{S} = \mathbf{H}^{-T} = (\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3 = \mathbf{p}) \ . \tag{29}$$

$\mathbf{f}_1$ and $\mathbf{f}_2$ are perpendicular to the ray, $\mathbf{f}_3$ equals slowness vector $\mathbf{p}$. Basis vectors $\mathbf{e}_i$ and $\mathbf{f}_i$ satisfy the relations,

$$\mathbf{e}_k^T \mathbf{f}_l = \delta_{kl} \ , \qquad \mathbf{e}_k \mathbf{f}_k^T = \mathbf{I} \ , \tag{30}$$

where $\mathbf{I}$ is the 3×3 identity matrix. Vectors $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ can be calculated from $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ using relations

$$\mathbf{f}_1 = \frac{(\mathbf{e}_2 \times \boldsymbol{\mathcal{U}})}{\boldsymbol{\mathcal{U}}^T(\mathbf{e}_1 \times \mathbf{e}_2)} \ , \quad \mathbf{f}_2 = \frac{(\boldsymbol{\mathcal{U}} \times \mathbf{e}_1)}{\boldsymbol{\mathcal{U}}^T(\mathbf{e}_1 \times \mathbf{e}_2)} \ , \quad \mathbf{f}_3 = \mathbf{p} \ . \tag{31}$$

Similarly, vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ can be calculated from $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ as follows:

$$\mathbf{e}_1 = \frac{(\mathbf{f}_2 \times \mathbf{p})}{\mathbf{p}^T(\mathbf{f}_1 \times \mathbf{f}_2)} \ , \quad \mathbf{e}_2 = \frac{(\mathbf{p} \times \mathbf{f}_1)}{\mathbf{p}^T(\mathbf{f}_1 \times \mathbf{f}_2)} \ , \quad \mathbf{e}_3 = \boldsymbol{\mathcal{U}} \ . \tag{32}$$

Similarly as in (3), we introduce two 3×1 matrices $\mathbf{Q}^{(q)} \equiv (Q_1^{(q)}, Q_2^{(q)}, Q_3^{(q)})^T$ and $\mathbf{P}^{(q)} \equiv (P_1^{(q)}, P_2^{(q)}, P_3^{(q)})^T$ along the ray,

$$\mathbf{Q}^{(q)} = \partial \mathbf{q} / \partial \gamma \ , \qquad \mathbf{P}^{(q)} = \partial \mathbf{p}^{(q)} / \partial \gamma \ , \tag{33}$$

where γ is an arbitrary ray parameter, and $\mathbf{p}^{(q)}$ is the slowness vector expressed in ray-centered coordinates,

$$p_i^{(q)} = \partial T / \partial q_i \ . \tag{34}$$

As $q_3 = \tau$, $p_3^{(q)} = 1$ along the reference ray. The superscript (q) indicates that the quantities are expressed in ray-centered coordinates.

The dynamic ray tracing system for smooth anisotropic inhomogeneous media in ray-centered coordinates for the 3×1 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$ was derived by Klimeš

(1994,2006), see also Červený (2001, sec. 4.2.4/3). It can be decoupled into two subsystems. The first subsystem for the 2×1 matrices $\boldsymbol{Q}^{(q)} \equiv (Q_1^{(q)}, Q_2^{(q)})^T$ and $\boldsymbol{P}^{(q)} \equiv (P_1^{(q)}, P_2^{(q)})^T$ consists of four equations

$$\begin{aligned} \mathrm{d}\boldsymbol{Q}^{(q)}/\mathrm{d}\tau &= \boldsymbol{A}^{(q)}\boldsymbol{Q}^{(q)} + \boldsymbol{B}^{(q)}\boldsymbol{P}^{(q)} \ , \\ \mathrm{d}\boldsymbol{P}^{(q)}/\mathrm{d}\tau &= -\boldsymbol{C}^{(q)}\boldsymbol{Q}^{(q)} - \boldsymbol{D}^{(q)}\boldsymbol{P}^{(q)} \ , \end{aligned} \tag{35}$$

where $\boldsymbol{A}^{(q)}$, $\boldsymbol{B}^{(q)}$, $\boldsymbol{C}^{(q)}$, and $\boldsymbol{D}^{(q)}$ are 2×2 matrices, calculated from the 3×3 matrices $\mathbf{A}^{(x)}$, $\mathbf{B}^{(x)}$, $\mathbf{C}^{(x)}$, and $\mathbf{D}^{(x)}$ as follows:

$$\begin{aligned} \boldsymbol{A}^{(q)} &= \mathbf{f}^T\mathbf{A}^{(x)}\mathbf{e} + \boldsymbol{d} \ , & \boldsymbol{B}^{(q)} &= \mathbf{f}^T\mathbf{B}^{(x)}\mathbf{f} \ , \\ \boldsymbol{C}^{(q)} &= \mathbf{e}^T(\mathbf{C}^{(x)} - \boldsymbol{\eta}^T\boldsymbol{\eta})\mathbf{e} \ , & \boldsymbol{D}^{(q)} &= \mathbf{e}^T\mathbf{D}^{(x)}\mathbf{f} - \boldsymbol{d}^T \ , \end{aligned} \tag{36}$$

and $\boldsymbol{d}$ is a 2×2 matrix given by the relation:

$$\boldsymbol{d} = \mathbf{f}^T\mathrm{d}\mathbf{e}/\mathrm{d}\tau \ . \tag{37}$$

Here the 3×3 matrices $\mathbf{A}^{(x)}$, $\mathbf{B}^{(x)}$, $\mathbf{C}^{(x)}$ and $\mathbf{D}^{(x)}$ are given by (5), and $\boldsymbol{\eta}$ by (2). Finally, $\mathbf{e}$ and $\mathbf{f}$ are 3×2 matrices,

$$\mathbf{e} = (\mathbf{e}_1, \mathbf{e}_2) \ , \qquad \mathbf{f} = (\mathbf{f}_1, \mathbf{f}_2) \ . \tag{38}$$

The second subsystem consists of two equations for $Q_3^{(q)}$ and $P_3^{(q)}$, and is extremely simple,

$$\mathrm{d}Q_3^{(q)}/\mathrm{d}\tau = P_3^{(q)} \ , \qquad \mathrm{d}P_3^{(q)}/\mathrm{d}\tau = 0 \ . \tag{39}$$

The analytic solution of (39) is

$$Q_3^{(q)}(\tau) = Q_3^{(q)}(\tau_0) + P_3^{(q)}(\tau_0)(\tau - \tau_0) \ , \quad P_3^{(q)}(\tau) = P_3^{(q)}(\tau_0) \ . \tag{40}$$

It should be noted that the constraint relation, analogous to (6), is trivial in ray-centered coordinates,

$$P_3^{(q)}(\tau) = 0 \ , \tag{41}$$

and, therefore, $Q_3^{(q)}(\tau)$ is constant along the ray in any smooth part of the medium. The constraint relation (41) applies to the subsystem (39) only. There is no constraint imposed on the subsystem (35).

Note that the DRT subsystem (35) remains valid even when $\boldsymbol{Q}^{(q)}$ and $\boldsymbol{P}^{(q)}$ represent 2×2 matrices

$$\boldsymbol{Q}^{(q)} = \begin{pmatrix} \partial q_1/\partial\gamma_1 & \partial q_1/\partial\gamma_2 \\ \partial q_2/\partial\gamma_1 & \partial q_2/\partial\gamma_2 \end{pmatrix} \ , \quad \boldsymbol{P}^{(q)} = \begin{pmatrix} \partial p_1^{(q)}/\partial\gamma_1 & \partial p_1^{(q)}/\partial\gamma_2 \\ \partial p_2^{(q)}/\partial\gamma_1 & \partial p_2^{(q)}/\partial\gamma_2 \end{pmatrix} \ , \tag{42}$$

where γ_1 and γ_2 are two ray parameters (corresponding to an orthonomic system of rays).

In isotropic inhomogeneous media, the arclength s along the reference ray Ω has been traditionally used as the q_3-coordinate in the ray-centered coordinate system $\mathbf{q} = (q_1, q_2, q_3)$; see Popov and Pšenčík (1978a,b), Červený, Klimeš and Pšenčík (1988). This choice does not influence the first subsystem (35) of the dynamic ray tracing system at all, but only its second subsystem (39). For more details, see Klimeš (2006).

Note that the equations for the transformation of $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$ across a structural interface, analogous to (16), i.e. the expressions for the interface propagator matrix $\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ in ray-centered coordinates, have not yet been published. They are, however, derived here as a by-product of our treatment, see Section 6.

Now we introduce the 6×6 ray propagator matrix $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates, corresponding to the DRT system (35) (with (42)) and (39). It has trivial entries in the third and sixth columns and rows. Using (39) – (41), we obtain

$$\mathbf{\Pi}^{(q)}(\tau,\tau_0) = \begin{pmatrix} \boldsymbol{Q}_1^{(q)}(\tau,\tau_0) & \boldsymbol{0} & \boldsymbol{Q}_2^{(q)}(\tau,\tau_0) & \boldsymbol{0} \\ \boldsymbol{0}^T & 1 & \boldsymbol{0}^T & \tau-\tau_0 \\ \boldsymbol{P}_1^{(q)}(\tau,\tau_0) & \boldsymbol{0} & \boldsymbol{P}_2^{(q)}(\tau,\tau_0) & \boldsymbol{0} \\ \boldsymbol{0}^T & 0 & \boldsymbol{0}^T & 1 \end{pmatrix} . \tag{43}$$

Here $\boldsymbol{Q}_1^{(q)}$ and $\boldsymbol{Q}_2^{(q)}$ are 2×2 matrices corresponding to $\boldsymbol{Q}^{(q)}$ in (42), and $\boldsymbol{P}_1^{(q)}$ and $\boldsymbol{P}_2^{(q)}$ are 2×2 matrices corresponding to $\boldsymbol{P}^{(q)}$ in (42), $\boldsymbol{0} = (0,0)^T$. For a detailed derivation of (43) see the pioneering paper by Klimeš (1994). Subscripts 1 and 2 of $\boldsymbol{Q}^{(q)}$ and $\boldsymbol{P}^{(q)}$ distinguish different initial conditions of $\boldsymbol{Q}_1^{(q)}$, $\boldsymbol{P}_1^{(q)}$ and of $\boldsymbol{Q}_2^{(q)}$, $\boldsymbol{P}_2^{(q)}$:

a) $\boldsymbol{Q}_1^{(q)}(\tau,\tau_0)$ and $\boldsymbol{P}_1^{(q)}(\tau,\tau_0)$ are 2×2 solutions of (35) with the plane-wavefront initial conditions at $\tau = \tau_0$:

$$\boldsymbol{Q}_1^{(q)} = \boldsymbol{I} , \qquad \boldsymbol{P}_1^{(q)} = \boldsymbol{0} . \tag{44}$$

b) $\boldsymbol{Q}_2^{(q)}(\tau,\tau_0)$ and $\boldsymbol{P}_2^{(q)}(\tau,\tau_0)$ are 2×2 solutions of (35) with the point source initial conditions at $\tau = \tau_0$:

$$\boldsymbol{Q}_2^{(q)} = \boldsymbol{0} , \qquad \boldsymbol{P}_2^{(q)} = \boldsymbol{I} . \tag{45}$$

As we can simply see from (43), the 4×4 ray propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau,\tau_0)$ in ray-centered coordinates q_1, q_2, corresponding to the DRT system (35) is given by the relation

$$\boldsymbol{\Pi}^{(q)}(\tau,\tau_0) = \begin{pmatrix} \boldsymbol{Q}_1^{(q)}(\tau,\tau_0) & \boldsymbol{Q}_2^{(q)}(\tau,\tau_0) \\ \boldsymbol{P}_1^{(q)}(\tau,\tau_0) & \boldsymbol{P}_2^{(q)}(\tau,\tau_0) \end{pmatrix} . \tag{46}$$

The 4×4 ray propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau,\tau_0)$ (46) is obtained from the 6×6 ray propagator matrix (43) by simply crossing the third and sixth columns and rows. The partial derivatives with respect to γ_1 and γ_2 in the 2×2 submatrices of $\boldsymbol{\Pi}^{(q)}(\tau,\tau_0)$ in (46) are taken for a fixed travel time $T = \tau$.

Analogously to (7)-(12), the 6×6 and 4×4 ray propagator matrices (43) and (46) in ray-centered coordinates satisfy the symplectic property, continuation property, chain property, etc. The continuation property for the 4×4 matrix (46) reads:

$$\begin{pmatrix} \boldsymbol{Q}^{(q)}(\tau) \\ \boldsymbol{P}^{(q)}(\tau) \end{pmatrix} = \boldsymbol{\Pi}^{(q)}(\tau,\tau_0) \begin{pmatrix} \boldsymbol{Q}^{(q)}(\tau_0) \\ \boldsymbol{P}^{(q)}(\tau_0) \end{pmatrix} , \tag{47}$$

which can also be expressed in the following form:

$$\begin{pmatrix} \delta\boldsymbol{q}(\tau) \\ \delta\boldsymbol{p}^{(q)}(\tau) \end{pmatrix} = \boldsymbol{\Pi}^{(q)}(\tau,\tau_0) \begin{pmatrix} \delta\boldsymbol{q}(\tau_0) \\ \delta\boldsymbol{p}^{(q)}(\tau_0) \end{pmatrix} , \tag{48}$$

Here the 2×1 vectors $\delta\boldsymbol{q}(\tau) \equiv (\delta q_1(\tau), \delta q_2(\tau))^T$ and $\delta\boldsymbol{p}^{(q)}(\tau) \equiv (\delta p_1^{(q)}(\tau), \delta p_2^{(q)}(\tau))^T$ are small perturbations of $\boldsymbol{q}$ and $\boldsymbol{p}^{(q)}$ around the reference ray Ω, measured along the plane tangent to the wavefront at Ω. They can also be expressed in terms of 2×2 matrices $\boldsymbol{Q}^{(q)}$ and $\boldsymbol{P}^{(q)}$ as follows:

$$\delta\boldsymbol{q} = \boldsymbol{Q}^{(q)}\delta\boldsymbol{\gamma} , \quad \delta\boldsymbol{p}^{(q)} = \boldsymbol{P}^{(q)}\delta\boldsymbol{\gamma} . \tag{49}$$

Here $\delta\boldsymbol{\gamma} \equiv (\gamma_1 - \gamma_{10}, \gamma_2 - \gamma_{20})^T$, and γ_{10}, γ_{20} are the ray parameters of the reference ray Ω.

In the solution of DRT system (35), it is necessary to know the basis vectors $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{f}_1, \mathbf{f}_2$ at any point of the reference ray Ω, see (36). These basis vectors can be calculated by solving ordinary differential equations of the first order along Ω. Actually, it is sufficient to calculate only one pair of basis vectors in this way, as the second pair can be obtained using (31) or (32). The relevant differential equations for $\mathbf{e}_1, \mathbf{e}_2$ contain only first-order derivatives of Hamiltonian, but for $\mathbf{f}_1, \mathbf{f}_2$ the second-order derivatives of Hamiltonian are needed. Consequently, it is simpler and more efficient to calculate $\mathbf{e}_1, \mathbf{e}_2$ by numerical integration along the ray, not $\mathbf{f}_1, \mathbf{f}_2$. It is common to take the ordinary differential equation of the first order for $\mathbf{e}_I, I = 1, 2$, as follows:

$$\mathrm{d}\mathbf{e}_I/\mathrm{d}\tau = -(\mathbf{p}^T\mathbf{p})^{-1}(\mathbf{e}_I^T\boldsymbol{\eta})\mathbf{p} . \tag{50}$$

where $\boldsymbol{\eta} = -\partial\mathcal{H}/\partial\mathbf{x}$, see (2). If we take $\mathbf{e}_1, \mathbf{e}_2$ as two vectors perpendicular to the slowness vector $\mathbf{p}$ at the initial point of the ray Ω, then (50) guarantees that $\mathbf{e}_1$ and $\mathbf{e}_2$ are perpendicular to $\mathbf{p}$ along the whole ray. The basis vectors $\mathbf{e}_1, \mathbf{e}_2$ need not be mutually perpendicular unit vectors. If we, however, take them mutually perpendicular and unit at the initial point of the ray, then (50) also guarantees that $\mathbf{e}_1$ and $\mathbf{e}_2$ have the same propecty along the whole ray. In such case, it is sufficient to solve (50) only for one vector of $\mathbf{e}_1$ and $\mathbf{e}_2$, and to compute the latter using the orthogonality condition of $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{p}$.

Let us now briefly compare the DRT systems (4) in Cartesian coordinates and (35) in ray-centered coordinates for anisotropic inhomogeneous medium. The DRT system (35) in ray-centered coordinates consists of four equations only, but the DRT system (4) in Cartesian coordinates of six equations. From the numerical point of view, this is a great advantage of DRT system (35). In other aspects, the DRT system (4) in Cartesian coordinates is simpler than that of (35). Actually, DRT system (4) uses only the 3×3 matrices $\mathbf{A}^{(x)}$, $\mathbf{B}^{(x)}$, $\mathbf{C}^{(x)}$ and $\mathbf{D}^{(x)}$, see (5). These matrices are needed even in DRT system (35), but system (35) also requires certain additional computations at each point of the ray. We shall list them briefly here:

1) In the solution of DRT system (35), it is necessary to know basis vectors $\mathbf{e}_1$, $\mathbf{e}_2$. These basis vectors should be calculated by numerical integration along the ray Ω, e.g. (50). The DRT system in Cartesian coordinates (4) does not require the computation of any basis vector.

2) If we determine $\mathbf{e}_1$ and $\mathbf{e}_2$ by numerical integration along the ray, e.g. using (50), we have to compute $\mathbf{f}_1$ and $\mathbf{f}_2$ using (31).

3) Further, we have to compute the 2×2 matrix $\boldsymbol{d}$. Using (37) and (50), we obtain for the components d_{NM} of $\boldsymbol{d}$:

$$d_{NM} = -(\mathbf{f}_N^T \mathbf{p})(\mathbf{e}_M^T \boldsymbol{\eta})/(\mathbf{p}^T \mathbf{p}) \ . \tag{51}$$

4) Only then can we perform the matrix multiplications in (36) and get $\boldsymbol{A}^{(q)}$, $\boldsymbol{B}^{(q)}$, $\boldsymbol{C}^{(q)}$ and $\boldsymbol{D}^{(q)}$.

Consequently, the conventional DRT system (4) in Cartesian coordinates is conceptually simpler and more straightforward than the DRT system (35) in ray-centered coordinates.

In practical applications, however, the 4×4 DRT propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates (46) is often more useful and physically more attractive than the 6×6 DRT propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates. The reason is that the general system of rays in smooth inhomogeneous media is four-parameteric, so that the number of equations corresponds strictly to the number of free parameters. In the 6×6 DRT propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates, two columns are redundant (ray-tangent and non-eikonal solutions) and must be removed.

In the following sections, we propose methods of avoiding the DRT in ray-centered coordinates (35) in the computation of the 4×4 ray propagator $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates. We determine $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ directly from $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$, without performing DRT (35) in ray-centered coordinates, and without the four computational steps (1)-(4) given above. We also show that it would be sufficient to compute only four columns of $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ if we wished to determine $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ from $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$.

4 Relation between ray propagator matrices $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ and $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$

A general relation between the 6×6 ray propagator matrices, computed along the same reference ray Ω from τ_0 to τ, related to two arbitrary coordinate systems, is given in Červený (2001), see eq. (4.3.38). In the equation, it is assumed that parameter τ along the ray is the same in both coordinate systems, and represents the travel time along the ray.

First we present the relations between the 3×1 matrices $\mathbf{Q}^{(x)}$, $\mathbf{P}^{(x)}$ and $\mathbf{Q}^{(q)}$, $\mathbf{P}^{(q)}$. A suitable form of these relations is given in Červený (2001, eq. 4.3.35). It reads:

$$\mathbf{Q}^{(q)} = \mathbf{H}^{-1}\mathbf{Q}^{(x)} \ , \quad \mathbf{P}^{(q)} = \mathbf{H}^T\mathbf{P}^{(x)} + \mathbf{F}\mathbf{H}^{-1}\mathbf{Q}^{(x)} \ . \tag{52}$$

Here $\mathbf{H}$ is the 3×3 transformation matrix given by (27), and $\mathbf{F}$ is a 3×3 symmetric matrix given by the relation

$$F_{mn} = p_i \frac{\partial^2 x_i}{\partial q_m \partial q_n} \ . \tag{53}$$

If we take into account (26), we obtain

$$F_{MN} = 0 \ , \quad F_{M3} = F_{3M} = -\mathbf{e}_M^T \boldsymbol{\eta} \ , \quad F_{33} = -\boldsymbol{\mathcal{U}}^T \boldsymbol{\eta} \ . \tag{54}$$

Relations (52) can be expressed in a more compact matrix form

$$\begin{pmatrix} \mathbf{Q}^{(q)} \\ \mathbf{P}^{(q)} \end{pmatrix} = \boldsymbol{\Psi}_1 \begin{pmatrix} \mathbf{Q}^{(x)} \\ \mathbf{P}^{(x)} \end{pmatrix} \ , \qquad \begin{pmatrix} \mathbf{Q}^{(x)} \\ \mathbf{P}^{(x)} \end{pmatrix} = \boldsymbol{\Psi}_2 \begin{pmatrix} \mathbf{Q}^{(q)} \\ \mathbf{P}^{(q)} \end{pmatrix} \ , \tag{55}$$

where $\boldsymbol{\Psi}_1$ and $\boldsymbol{\Psi}_2$ are 6×6 matrices, given by the relations

$$\boldsymbol{\Psi}_1 = \begin{pmatrix} \mathbf{H}^{-1} & \mathbf{0} \\ \mathbf{F}\mathbf{H}^{-1} & \mathbf{H}^T \end{pmatrix} \ , \qquad \boldsymbol{\Psi}_2 = \begin{pmatrix} \mathbf{H} & \mathbf{0} \\ -\mathbf{H}^{-T}\mathbf{F} & \mathbf{H}^{-T} \end{pmatrix} \ , \tag{56}$$

and $\mathbf{0}$ is a 3×3 null matrix. Obviously, $\boldsymbol{\Psi}_1 \boldsymbol{\Psi}_2 = \mathbf{I}$. Both matrices $\boldsymbol{\Psi}_1$ and $\boldsymbol{\Psi}_2$ are symplectic.

To express $\boldsymbol{\Psi}_1$ and $\boldsymbol{\Psi}_2$ in a more suitable form, we introduce a 3×3 matrix $\mathbf{V}$,

$$\mathbf{V} = \mathbf{H}^{-T}\mathbf{F} \ . \tag{57}$$

The columns of matrix $\mathbf{V}$ are given by expressions

$$\mathbf{V}_1 = -(\mathbf{e}_1^T \boldsymbol{\eta})\mathbf{p} \ , \quad \mathbf{V}_2 = -(\mathbf{e}_2^T \boldsymbol{\eta})\mathbf{p} \ , \quad \mathbf{V}_3 = -(\mathbf{e}_m^T \boldsymbol{\eta})\mathbf{f}_m \ . \tag{58}$$

The 6×6 matrices $\boldsymbol{\Psi}_1$ and $\boldsymbol{\Psi}_2$ then read

$$\boldsymbol{\Psi}_1 = \begin{pmatrix} \mathbf{f}^T & \mathbf{0} \\ \mathbf{V}^T & \mathbf{e}^T \end{pmatrix} \ , \qquad \boldsymbol{\Psi}_2 = \begin{pmatrix} \mathbf{e} & \mathbf{0} \\ -\mathbf{V} & \mathbf{f} \end{pmatrix} \ , \tag{59}$$

where $\mathbf{V} \equiv (\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3)$.

Now we derive the transformation between the 6×6 ray propagator matrices $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ and $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$. Multiplying (9) from the left by $\boldsymbol{\Psi}_1(\tau)$, and using the second equation of (55) for τ_0, we obtain

$$\begin{pmatrix} \mathbf{Q}^{(q)}(\tau) \\ \mathbf{P}^{(q)}(\tau) \end{pmatrix} = \boldsymbol{\Psi}_1(\tau)\mathbf{\Pi}^{(x)}(\tau, \tau_0)\boldsymbol{\Psi}_2(\tau_0) \begin{pmatrix} \mathbf{Q}^{(q)}(\tau_0) \\ \mathbf{P}^{(q)}(\tau_0) \end{pmatrix} \ . \tag{60}$$

This implies that the 6×6 ray propagator matrix $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates can be expressed in terms of the 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates as follows:

$$\mathbf{\Pi}^{(q)}(\tau, \tau_0) = \boldsymbol{\Psi}_1(\tau)\mathbf{\Pi}^{(x)}(\tau, \tau_0)\boldsymbol{\Psi}_2(\tau_0) \ . \tag{61}$$

This is the final transformation relation between the 6×6 ray propagator matrices $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ and $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$. It also follows from the general expression given in Červený (2001, eq.(4.3.38)).

Equation (61) can be simply modified to yield a 4×4 ray propagator matrix $\boldsymbol{\mathit{\Pi}}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates q_1, q_2, corresponding to DRT system (35). We simply remove the third and sixth columns in $\boldsymbol{\Psi}_2$ and third and sixth rows in $\boldsymbol{\Psi}_1$. We obtain

$$\boldsymbol{\mathit{\Pi}}^{(q)}(\tau, \tau_0) = \boldsymbol{\Psi}_1^r(\tau)\mathbf{\Pi}^{(x)}(\tau, \tau_0)\boldsymbol{\Psi}_2^r(\tau_0) \ . \tag{62}$$

The "reduced" matrices $\mathbf{\Psi}_1^r$ and $\mathbf{\Psi}_2^r$ are 4×6 and 6×4, respectively, and are given by relations

$$\mathbf{\Psi}_1^r = \begin{pmatrix} \mathbf{f}_1^T & \mathbf{0}^T \\ \mathbf{f}_2^T & \mathbf{0}^T \\ \mathbf{V}_1^T & \mathbf{e}_1^T \\ \mathbf{V}_2^T & \mathbf{e}_2^T \end{pmatrix} , \quad \mathbf{\Psi}_2^r = \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{0} & \mathbf{0} \\ -\mathbf{V}_1 & -\mathbf{V}_2 & \mathbf{f}_1 & \mathbf{f}_2 \end{pmatrix} . \tag{63}$$

Here $\mathbf{0} = (0,0,0)^T$. The reduced matrices $\mathbf{\Psi}_1^r$ and $\mathbf{\Psi}_2^r$ again satisfy the relation $\mathbf{\Psi}_1^r \mathbf{\Psi}_2^r = \mathbf{I}$, where $\mathbf{I}$ is a 4×4 identity matrix.

The relations (61) and (62) are valid for arbitrarily chosen contravariant basis vector $\mathbf{e}_1(\tau_0)$ and $\mathbf{e}_2(\tau_0)$, situated in the wavefront tangent plane at τ_0, and covariant basis vector $\mathbf{f}_1(\tau_0)$, $\mathbf{f}_2(\tau_0)$, situated in the plane perpendicular to the reference ray Ω, satisfying the relation (30). Note that $\mathbf{e}_3(\tau_0) = \boldsymbol{\mathcal{U}}(\tau_0)$ and $\mathbf{f}_3(\tau_0) = \mathbf{p}(\tau_0)$. Similarly, the choice of $\mathbf{e}_1(\tau)$, $\mathbf{e}_2(\tau)$, $\mathbf{f}_1(\tau)$, and $\mathbf{f}_2(\tau)$ is also arbitrary, they only must satisfy (30), with $\mathbf{e}_3(\tau) = \boldsymbol{\mathcal{U}}(\tau)$ and $\mathbf{f}_3(\tau) = \mathbf{p}(\tau)$. Thus, the numerical integration of (50) is not required in this case, and relations (48) with (62) can be safely used to compute $\delta\boldsymbol{q}(\tau)$ and $\delta\boldsymbol{p}^{(q)}(\tau)$ from $\delta\boldsymbol{q}(\tau_0)$ and $\delta\boldsymbol{p}^{(q)}(\tau_0)$, for $\mathbf{e}_1(\tau_0)$, $\mathbf{e}_2(\tau_0)$ and $\mathbf{e}_1(\tau)$, $\mathbf{e}_2(\tau)$ arbitrarily and independently specified.

Equation (62), however, gives the 4×4 propagator matrix in ray-centered coordinates only if $\boldsymbol{\Pi}^{(q)}(\tau_0, \tau_0) = \boldsymbol{I}$, where $\boldsymbol{I}$ is a 4×4 identity matrix. This is guaranteed only if $\mathbf{\Psi}_1^r(\tau) \to \mathbf{\Psi}_1^r(\tau_0)$ for $\tau \to \tau_0$, see (61). In such case, a solution of (50) (or some other analogous equation) is needed.

5 Alternative computation of $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$

We now use an alternative approach to determine $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$, proposed by Klimeš (1994). The advantage of this approach is that it does not require six dynamic ray tracings in Cartesian coordinates, but only four, for some selected initial conditions. The remaining two solutions of the dynamic ray tracing system in Cartesian coordinates are known explicitly (ray tangent solutions, non-eikonal solutions).

We can proceed in the following way. We express (61) as follows:

$$\mathbf{\Pi}^{(q)}(\tau, \tau_0) = \mathbf{\Psi}_1(\tau) \mathbf{Z}(\tau, \tau_0) , \tag{64}$$

where

$$\mathbf{Z}(\tau, \tau_0) = \mathbf{\Pi}^{(x)}(\tau, \tau_0) \mathbf{\Psi}_2(\tau_0) . \tag{65}$$

The 6×6 matrix $\mathbf{Z}(\tau, \tau_0)$ is not a propagator matrix, as $\mathbf{Z}(\tau_0, \tau_0) = \mathbf{\Psi}_2(\tau_0)$ is different from identity matrix $\mathbf{I}$. The six columns of $\mathbf{Z}(\tau, \tau_0)$ are the solutions of the dynamic ray tracing system (4) in Cartesian coordinates, with initial conditions given by $\mathbf{\Psi}_2(\tau_0)$.

Two of the solutions of the dynamic ray tracing system in Cartesian coordinates, however, are known analytically. This is the ray-tangent solution, see (13), and the non-eikonal solution (14). Conventionally, we store the ray tangent solution (13) in the third column of $\mathbf{Z}(\tau, \tau_0)$, and the non-eikonal solution (14) in its sixth column. The remaining columns represent standard paraxial solutions of the DRT in Cartesian coordinates, with the initial condition given in the relevant column of $\mathbf{\Psi}_2(\tau_0)$. The standard paraxial solutions in $\mathbf{Z}(\tau,\tau_0)$ must satisfy the constraint equation (6). Moreover, $\mathbf{Q}^{(x)}$ must satisfy the relation

$$\mathbf{p}^T\mathbf{Q}^{(x)} = 0 \ , \tag{66}$$

expressing the fact that vector $\mathbf{Q}^{(x)}$ is tangent to the wavefront at the reference ray.

Now we shall compute $\mathbf{\Pi}^{(q)}(\tau,\tau_0)$ using Eq. (64). First we compute the product of $\mathbf{\Psi}_1$, given by (59), with the third and sixth columns of $\mathbf{Z}(\tau,\tau_0)$, representing the ray-tangent and non-eikonal solutions (13) and (14). For the ray-tangent solutions, (59) and (13) yield

$$\mathbf{\Psi}_1 \begin{pmatrix} \boldsymbol{\mathcal{U}} \\ \boldsymbol{\eta} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1^T\boldsymbol{\mathcal{U}} \\ \mathbf{f}_2^T\boldsymbol{\mathcal{U}} \\ \mathbf{f}_3^T\boldsymbol{\mathcal{U}} \\ -(\mathbf{e}_1^T\boldsymbol{\eta})(\mathbf{p}^T\boldsymbol{\mathcal{U}}) + \mathbf{e}_1^T\boldsymbol{\eta} \\ -(\mathbf{e}_2^T\boldsymbol{\eta})(\mathbf{p}^T\boldsymbol{\mathcal{U}}) + \mathbf{e}_2^T\boldsymbol{\eta} \\ -\boldsymbol{\eta}^T\boldsymbol{\mathcal{U}} + \mathbf{e}_3^T\boldsymbol{\eta} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} . \tag{67}$$

Here we have taken into account that $\mathbf{f}_I^T\boldsymbol{\mathcal{U}} = 0$, $\mathbf{p}^T\boldsymbol{\mathcal{U}} = 1$ and $\mathbf{f}_3^T\boldsymbol{\mathcal{U}} = \mathbf{p}^T\boldsymbol{\mathcal{U}} = 1$. Similarly, for the non-eikonal solution, (59) and (14) yield

$$\mathbf{\Psi}_1 \begin{pmatrix} \boldsymbol{\mathcal{U}}\Delta\tau \\ \mathbf{p} + \boldsymbol{\eta}\Delta\tau \end{pmatrix} = \begin{pmatrix} \Delta\tau(\mathbf{f}_1^T\boldsymbol{\mathcal{U}}) \\ \Delta\tau(\mathbf{f}_2^T\boldsymbol{\mathcal{U}}) \\ \Delta\tau(\mathbf{f}_3^T\boldsymbol{\mathcal{U}}) \\ -\Delta\tau(\mathbf{e}_1^T\boldsymbol{\mathcal{U}})(\mathbf{p}^T\boldsymbol{\mathcal{U}}) + \mathbf{e}_1^T\mathbf{p} + \Delta\tau(\mathbf{e}_1^T\boldsymbol{\eta}) \\ -\Delta\tau(\mathbf{e}_2^T\boldsymbol{\mathcal{U}})(\mathbf{p}^T\boldsymbol{\mathcal{U}}) + \mathbf{e}_2^T\mathbf{p} + \Delta\tau(\mathbf{e}_2^T\boldsymbol{\eta}) \\ -\Delta\tau(\boldsymbol{\eta}^T\boldsymbol{\mathcal{U}}) + \mathbf{e}_3^T\mathbf{p} + \Delta\tau(\mathbf{e}_3^T\boldsymbol{\eta}) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \Delta\tau \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{68}$$

Here $\Delta\tau$ stands for $\tau - \tau_0$.

Thus, the third and sixth columns of $\mathbf{\Pi}^{(q)}(\tau,\tau_0)$ are given by simple expressions (67) and (68).

We shall now consider the standard paraxial solutions (the first, second, fourth and fifth columns) of $\mathbf{Z}(\tau,\tau_0)$. We denote any of them

$$\begin{pmatrix} \mathbf{Q}^{(x)} \\ \mathbf{P}^{(x)} \end{pmatrix} , \tag{69}$$

where $\mathbf{Q}^{(x)} \equiv (Q_1^{(x)}, Q_2^{(x)}, Q_3^{(x)})^T$ and $\mathbf{P}^{(x)} \equiv (P_1^{(x)}, P_2^{(x)}, P_3^{(x)})^T$. The product of matrix $\mathbf{\Psi}_1$ with any of the solutions (69) reads

$$\mathbf{\Psi}_1 \begin{pmatrix} \mathbf{Q}^{(x)} \\ \mathbf{P}^{(x)} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1^T\mathbf{Q}^{(x)} \\ \mathbf{f}_2^T\mathbf{Q}^{(x)} \\ \mathbf{f}_3^T\mathbf{Q}^{(x)} \\ -(\mathbf{e}_1^T\boldsymbol{\eta})(\mathbf{p}^T\mathbf{Q}^{(x)}) + \mathbf{e}_1^T\mathbf{P}^{(x)} \\ -(\mathbf{e}_2^T\boldsymbol{\eta})(\mathbf{p}^T\mathbf{Q}^{(x)}) + \mathbf{e}_2^T\mathbf{P}^{(x)} \\ -\boldsymbol{\eta}^T\mathbf{Q}^{(x)} + \mathbf{e}_3^T\mathbf{P}^{(x)} \end{pmatrix} = \begin{pmatrix} \times \\ \times \\ 0 \\ \times \\ \times \\ 0 \end{pmatrix} . \tag{70}$$

The crosses $\times$ denote possibly non-zero entries. The zero in the third row follows immediately from (66), and the zero in the sixth row from the relation $(\mathbf{e}_m^T\boldsymbol{\eta})(\mathbf{f}_m^T\mathbf{Q}^{(x)}) = \boldsymbol{\eta}^T\mathbf{Q}^{(x)}$ and from the constraint relation (6).

Thus, the 6×6 ray propagator matrix $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates takes a specific form: It has zero values in the third and sixth columns and rows, with the exception of positions 33 and 66, where it is 1, and of position 36, where it equals $\tau - \tau_0$. Consequently, it can be expressed in the form of (43). This provides an independent derivation of the specific form of (43).

From the 6×6 ray propagator matrix $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ given by (64), we can again obtain the 4×4 ray propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ as follows:

$$\boldsymbol{\Pi}^{(q)}(\tau, \tau_0) = \mathbf{\Psi}_1^r(\tau)\mathbf{Z}^r(\tau, \tau_0) \ . \tag{71}$$

Here $\mathbf{\Psi}_1^r$ corresponds to $\mathbf{\Psi}_1$ given by (59), in which the third and sixth rows have been removed, see (63). Similarly, $\mathbf{Z}^r(\tau, \tau_0)$ ($\mathbf{Z}$-reduced) contains four solutions of the DRT system in Cartesian coordinates (4) along the reference ray, from the initial point τ_0 to τ. These four solutions are specified by the initial conditions given by the 6×4 matrix $\mathbf{\Psi}_2^r(\tau_0)$ ($\mathbf{\Psi}_2$-reduced), see (63),

$$\mathbf{\Psi}_2^r(\tau_0) = \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{0} & \mathbf{0} \\ (\mathbf{e}_1^T\boldsymbol{\eta})\mathbf{p} & (\mathbf{e}_2^T\boldsymbol{\eta})\mathbf{p} & \mathbf{f}_1 & \mathbf{f}_2 \end{pmatrix} \ . \tag{72}$$

The first two columns in $\mathbf{\Psi}_2^r(\tau_0)$ correspond to the plane wavefront initial conditions

$$\mathbf{\Psi}^{pw}(\tau_0) = \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 \\ (\mathbf{e}_1^T\boldsymbol{\eta})\mathbf{p} & (\mathbf{e}_2^T\boldsymbol{\eta})\mathbf{p} \end{pmatrix} \ , \tag{73}$$

and the third and fourth column correspond to the point source initial condition

$$\mathbf{\Psi}^{ps}(\tau_0) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{f}_1 & \mathbf{f}_2 \end{pmatrix} \ . \tag{74}$$

Exactly the same initial conditions as (73) and (74) were also derived in Červený (2001, eqs. (4.2.50) – (4.2.52)), in relation to wavefront orthonormal coordinates. To compare (74) for a point source with (4.2.51) of Červený (2001), we can take into account that $\mathbf{f}_I$, given by (31), can also be expressed in the form: $\mathbf{f}_I = \mathbf{e}_I - \mathbf{p}(\mathbf{e}_I^T\boldsymbol{\mathcal{U}})$, if $\mathbf{e}_1$ and $\mathbf{e}_2$ are mutually perpendicular unit vectors. Equations fully analogous to (74) with the above expression for $\mathbf{f}_I$ were also derived by Pšenčík and Teles (1996).

Equation (71) represents the final result of this section. It expresses the 4×4 ray propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates, in terms of the 6×4 matrix $\mathbf{Z}^r(\tau, \tau_0)$, composed of four solutions of the dynamic ray tracing system in Cartesian coordinates, with initial conditions specified by matrix $\mathbf{\Psi}_2^r(\tau_0)$, given by (72). Dynamic ray tracing in ray-centered coordinates is not necessary. Similarly, the non-eikonal and ray tangent solutions are not needed.

6 Interface propagator matrix in ray-centered coordinates

We shall now apply (61) to compute the 6×6 interface propagator matrix $\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ in ray-centered coordinates from the 6×6 interface propagator matrix $\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ (17) in

Cartesian coordinates. We obtain

$$\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\boldsymbol{\Psi}_1(\tilde{\tau}_\Sigma)\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma,\tau_\Sigma)\boldsymbol{\Psi}_2(\tau_\Sigma)\ . \tag{75}$$

Here $\boldsymbol{\Psi}_1$ and $\boldsymbol{\Psi}_2$ are given by (59), and $\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma,\tau_\Sigma)$ by (17). Mostly, however, only the 2×2 matrices $\boldsymbol{Q}^{(q)}$ and $\boldsymbol{P}^{(q)}$ are used. The relevant 4×4 interface propagator matrix $\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)$ in ray-centered coordinates then reads

$$\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\boldsymbol{\Psi}_1^r(\tilde{\tau}_\Sigma)\mathbf{\Pi}^{(x)}(\tilde{\tau}_\Sigma,\tau_\Sigma)\boldsymbol{\Psi}_2^r(\tau_\Sigma)\ , \tag{76}$$

where the 4×6 matrix $\boldsymbol{\Psi}_1^r$ and the 6×4 matrix $\boldsymbol{\Psi}_2^r$ are given by (63).

Consequently, Equations (75) and (76) provide the possibility of performing the dynamic ray tracing (35) in ray-centered coordinates even for anisotropic inhomogeneous media with structural interfaces.

We now express the 6×6 interface propagator matrix $\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)$ (75) in a more compact form. Using (17) and (56), we obtain from (75),

$$\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\begin{pmatrix}\tilde{\mathbf{H}}^{-1} & \mathbf{0}\\ \tilde{\mathbf{F}}\tilde{\mathbf{H}}^{-1} & \tilde{\mathbf{H}}^T\end{pmatrix}\begin{pmatrix}\tilde{\mathbf{X}}\mathbf{X}^{-1} & \mathbf{0}\\ \tilde{\mathbf{X}}^{-T}\mathbf{R}\mathbf{X}^{-1} & \tilde{\mathbf{X}}^{-T}\mathbf{X}^T\end{pmatrix}\begin{pmatrix}\mathbf{H} & \mathbf{0}\\ -\mathbf{H}^T\mathbf{F} & \mathbf{H}^{-T}\end{pmatrix}\ . \tag{77}$$

This yields,

$$\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\begin{pmatrix}\tilde{\mathbf{K}}^T\mathbf{K}^{-T} & \mathbf{0}\\ \tilde{\mathbf{K}}^{-1}\mathbf{R}\mathbf{K}^{-T}+\tilde{\mathbf{F}}\tilde{\mathbf{K}}^T\mathbf{K}^{-T}-\tilde{\mathbf{K}}^{-1}\mathbf{K}\mathbf{F} & \tilde{\mathbf{K}}^{-1}\mathbf{K}\end{pmatrix}\ , \tag{78}$$

where

$$\mathbf{K}=\mathbf{X}^T\mathbf{H}^{-T}\ ,\qquad \tilde{\mathbf{K}}=\tilde{\mathbf{X}}^T\tilde{\mathbf{H}}^{-T}\ . \tag{79}$$

Equation (78) can also be expressed in a more symmetrical form

$$\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\begin{pmatrix}\tilde{\mathbf{K}}^T\mathbf{K}^{-T} & \mathbf{0}\\ \tilde{\mathbf{K}}^{-1}(\mathbf{R}+\tilde{\mathbf{K}}\tilde{\mathbf{F}}\tilde{\mathbf{K}}^T-\mathbf{K}\mathbf{F}\mathbf{K}^T)\mathbf{K}^{-T} & \tilde{\mathbf{K}}^{-1}\mathbf{K}\end{pmatrix}\ , \tag{80}$$

It may be useful to express $\mathbf{H}^{-T}$ and $\mathbf{K}^{-T}$ explicitly, $\mathbf{H}^{-T}=\mathbf{S}$ and $\mathbf{X}^{-T}=\mathbf{U}$, see (20) and (29). Then we obtain

$$\begin{aligned}&\mathbf{K}=\mathbf{X}^T\mathbf{H}^{-T}=\mathbf{X}^T\mathbf{S}\ , && \mathbf{K}^T=\mathbf{H}^{-1}\mathbf{X}=\mathbf{S}^T\mathbf{X}\ ,\\ &\mathbf{K}^{-1}=\mathbf{H}^T\mathbf{X}^{-T}=\mathbf{H}^T\mathbf{U}\ , && \mathbf{K}^{-T}=\mathbf{X}^{-1}\mathbf{H}=\mathbf{U}^T\mathbf{H}\ ,\end{aligned} \tag{81}$$

and similarly for the tilded quantities. Consequently, all 3×3 matrices $\mathbf{K},\mathbf{K}^T,\mathbf{K}^{-1}$ and $\mathbf{K}^{-T}$ are expressed in terms of scalar products of the basis vectors of the ray-centered coordinate system and the basis vectors of the local coordinate system at interface Σ. As will be explained below, this gives a clear physical meaning to all matrices $\mathbf{K},\mathbf{K}^T,\mathbf{K}^{-1}$ and $\mathbf{K}^{-T}$.

We can also replace matrix $\mathbf{F}$ by $\mathbf{V}$ using (57),

$$\mathbf{K}\mathbf{F}\mathbf{K}^T=\mathbf{X}^T\mathbf{H}^{-T}\mathbf{F}\mathbf{K}^T=\mathbf{X}^T\mathbf{V}\mathbf{K}^T\ , \tag{82}$$

and similarly for $\tilde{\mathbf{K}}\tilde{\mathbf{F}}\tilde{\mathbf{K}}^T$.

It is simple to show that the 3×3 matrices $\mathbf{K}, \mathbf{K}^{-1}, \mathbf{K}^T$ and $\mathbf{K}^{-T}$ have a special form. The third columns of matrices $\mathbf{K}^T$ and $\mathbf{K}^{-T}$ are $(0,0,1)^T$, and the third rows of $\mathbf{K}$ and $\mathbf{K}^{-1}$ are $(0,0,1)$. This follows from the property that basis vectors $\mathbf{f}_1, \mathbf{f}_2, \mathbf{h}_1$ and $\mathbf{h}_2$ are perpendicular to $\boldsymbol{\mathcal{U}}$, and that $\mathbf{p}^T\boldsymbol{\mathcal{U}} = \mathbf{h}_3^T\boldsymbol{\mathcal{U}} = 1$. Analogous properties are valid also for the tilded quantities. The partition matrices $\tilde{\mathbf{K}}^T\mathbf{K}^{-1}$ and $\tilde{\mathbf{K}}^{-1}\mathbf{K}$ in (80) have a similar form: the third column of $\tilde{\mathbf{K}}^T\mathbf{K}^{-1}$ is $(0,0,1)^T$, and the third row of $\tilde{\mathbf{K}}^{-1}\mathbf{K}$ is $(0,0,1)$. In addition, all elements of the third row and third column of the 3×3 matrix $\mathbf{R} + \tilde{\mathbf{K}}\tilde{\mathbf{F}}\tilde{\mathbf{K}}^T - \mathbf{K}\mathbf{F}\mathbf{K}^T$, and consequently of $\tilde{\mathbf{K}}^{-1}(\mathbf{R} + \tilde{\mathbf{K}}\tilde{\mathbf{F}}\tilde{\mathbf{K}}^T - \mathbf{K}\mathbf{F}\mathbf{K}^T)\mathbf{K}^{-T}$, vanish.

Then we can express the 6×6 interface propagator matrix in ray-centered coordinates as follows:

$$\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma) = \begin{pmatrix} \tilde{\boldsymbol{K}}^T \boldsymbol{K}^{-T} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{A}^T & 1 & \boldsymbol{0}^T & 0 \\ \tilde{\boldsymbol{K}}^{-1}[\boldsymbol{E} - \tilde{\boldsymbol{E}} - (\sigma - \tilde{\sigma})\boldsymbol{D}]\boldsymbol{K}^{-T} & \boldsymbol{0} & \tilde{\boldsymbol{K}}^{-1}\boldsymbol{K} & \boldsymbol{B} \\ \boldsymbol{0}^T & 0 & \boldsymbol{0}^T & 1 \end{pmatrix} . \tag{83}$$

Here $\boldsymbol{K}, \boldsymbol{K}^T, \boldsymbol{K}^{-1}$ and $\boldsymbol{K}^{-T}$ are the 2×2 upper left submatrices of the 3×3 matrices $\mathbf{K}, \mathbf{K}^T, \mathbf{K}^{-1}$ and $\mathbf{K}^{-T}$, respectively. They are expressed as scalar products of the basis vectors as follows:

$$\begin{aligned} \boldsymbol{K} &= (\mathbf{g}_1, \mathbf{g}_2)^T(\mathbf{f}_1, \mathbf{f}_2) , & \boldsymbol{K}^T &= (\mathbf{f}_1, \mathbf{f}_2)^T(\mathbf{g}_1, \mathbf{g}_2) , \\ \boldsymbol{K}^{-1} &= (\mathbf{e}_1, \mathbf{e}_2)^T(\mathbf{h}_1, \mathbf{h}_2) , & \boldsymbol{K}^{-T} &= (\mathbf{h}_1, \mathbf{h}_2)^T(\mathbf{e}_1, \mathbf{e}_2) . \end{aligned} \tag{84}$$

The scalar quantities σ and $\tilde{\sigma}$ represent the components of slowness vectors $\mathbf{p}$ and $\tilde{\mathbf{p}}$ into $\mathbf{n}^\Sigma$, $\sigma = \mathbf{p}^T\mathbf{n}^\Sigma$ and $\tilde{\sigma} = \tilde{\mathbf{p}}^T\mathbf{n}^\Sigma$. The 2×2 *curvature matrix* $\boldsymbol{D}$ is given by its elements

$$D_{IJ} = \mathbf{g}_{IJ}^T\mathbf{n}^\Sigma , \tag{85}$$

Note that $\boldsymbol{D} = \boldsymbol{0}$ for plane surface Σ. The 2×2 *inhomogeneity matrix* $\boldsymbol{E}$ is given by elements:

$$E_{IJ} = (\mathbf{g}_I^T\mathbf{p})(\mathbf{e}_K^T\boldsymbol{\eta})(\mathbf{g}_J^T\mathbf{f}_K) + (\mathbf{g}_I^T\boldsymbol{\eta})(\mathbf{g}_J^T\mathbf{p}) . \tag{86}$$

Matrix $\tilde{\boldsymbol{E}}$ is quite analogous. Note that $\boldsymbol{E} = \boldsymbol{0}$ for homogeneous media, as $\boldsymbol{\eta} = \mathbf{0}$ there. Here and above, $\boldsymbol{0}$ is a 2×1 or 2×2 zero matrix.

It remains to give the expressions for the 2×1 matrices $\boldsymbol{A} = (A_1, A_2)^T$ and $\boldsymbol{B} = (B_1, B_2)^T$:

$$A_I = (\mathbf{e}_I^T\mathbf{h}_K)(\mathbf{g}_K^T\mathbf{p}) + (\mathbf{e}_I^T\mathbf{h}_3) , \quad B_I = (\tilde{\mathbf{e}}_I^T\tilde{\mathbf{h}}_K)(\mathbf{g}_K^T\tilde{\mathbf{p}}) + (\tilde{\mathbf{e}}_I^T\tilde{\mathbf{h}}_3) . \tag{87}$$

In fact, it is easy to show that $\boldsymbol{A}$ and $\boldsymbol{B}$ are $\boldsymbol{0}$. As $\mathbf{g}_3^T\mathbf{p} = 1$, we obtain from (87)

$$A_I = \mathbf{e}_I^T\mathbf{h}_K\mathbf{g}_K^T\mathbf{p} + \mathbf{e}_I^T\mathbf{h}_3\mathbf{g}_3^T\mathbf{p} = \mathbf{e}_I^T\mathbf{h}_k\mathbf{g}_k^T\mathbf{p} = \boldsymbol{0} . \tag{88}$$

Here we have used $\mathbf{h}_k\mathbf{g}_k^T = \mathbf{I}$, see (24), and $\mathbf{e}_I^T\mathbf{p} = 0$. Quite analogously, we obtain $B_I = 0$. Consequently, the final expression for the 6×6 interface propagator matrix $\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$

in ray-centered coordinates reads:

$$\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\begin{pmatrix} \tilde{\boldsymbol{K}}^T\boldsymbol{K}^{-T} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0}^T & 1 & \boldsymbol{0}^T & 0 \\ \tilde{\boldsymbol{K}}^{-1}[\boldsymbol{E}-\tilde{\boldsymbol{E}}-(\sigma-\tilde{\sigma})\boldsymbol{D}]\boldsymbol{K}^{-T} & \boldsymbol{0} & \tilde{\boldsymbol{K}}^{-1}\boldsymbol{K} & \boldsymbol{0} \\ \boldsymbol{0}^T & 0 & \boldsymbol{0}^T & 1 \end{pmatrix} . \tag{89}$$

The 6×6 interface propagator matrix (89) in ray-centered coordinates is symplectic, and its determinant equals unity. The continuation property across interface Σ then reads:

$$\begin{pmatrix} \tilde{\boldsymbol{Q}}^{(q)} \\ \tilde{Q}_3^{(q)} \\ \tilde{\boldsymbol{P}}^{(q)} \\ \tilde{P}_3^{(q)} \end{pmatrix} = \mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)\begin{pmatrix} \boldsymbol{Q}^{(q)} \\ Q_3^{(q)} \\ \boldsymbol{P}^{(q)} \\ P_3^{(q)} \end{pmatrix} , \tag{90}$$

where $\mathbf{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)$ is a 6×6 matrix given by (89), $\boldsymbol{Q}^{(q)}\equiv(Q_1^{(q)},Q_2^{(q)})^T$ and $\boldsymbol{P}^{(q)}\equiv(P_1^{(q)},P_2^{(q)})^T$. The sixth line of (89) indicates that the interface propagator matrix preserves the constraint relation $P_3^{(q)}=0$ even across the interface, see (41). Similarly, the third line of (89) shows that $Q_3^{(q)}$ remains constant across the interface. Further, $\tilde{\boldsymbol{Q}}^{(q)}$ and $\tilde{\boldsymbol{P}}^{(q)}$ do not depend on $Q_3^{(q)}$.

Consequently, we can introduce the 4×4 interface propagator matrix in ray-centered coordinates $\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)$:

$$\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)=\begin{pmatrix} \tilde{\boldsymbol{K}}^T\boldsymbol{K}^{-T} & \boldsymbol{0} \\ \tilde{\boldsymbol{K}}^{-1}(\boldsymbol{E}-\tilde{\boldsymbol{E}}-(\sigma-\tilde{\sigma})\boldsymbol{D})\boldsymbol{K}^{-T} & \tilde{\boldsymbol{K}}^{-1}\boldsymbol{K} \end{pmatrix} . \tag{91}$$

The continuation property for $\boldsymbol{Q}^{(q)}$ and $\boldsymbol{P}^{(q)}$ then reads:

$$\begin{pmatrix} \tilde{\boldsymbol{Q}}^{(q)} \\ \tilde{\boldsymbol{P}}^{(q)} \end{pmatrix} = \boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)\begin{pmatrix} \boldsymbol{Q}^{(q)} \\ \boldsymbol{P}^{(q)} \end{pmatrix} . \tag{92}$$

Equations (91) and (92) represent the final results of this section. It would be possible to derive them directly from (76). We, however, wished to explain the physical arguments leading to the simplification of the 6×6 to 4×4 matrices. For this reason, we started the derivation from Equation (75).

The 4×4 interface propagator matrix $\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma,\tau_\Sigma)$ in ray-centered coordinates, given by (91), is symplectic, and the determinant of (91) equals unity. Basis vectors $\mathbf{g}_1$ and $\mathbf{g}_2$ are tangent to surface Σ, but need not to be unit or mutually perpendicular. Similarly, $\mathbf{n}^\Sigma$ is perpendicular to Σ, but need not be unit.

The 4×4 interface propagator matrix (91) in ray-centered coordinates is expressed in a form similar to the 4×4 interface propagator matrix in wavefront orthonormal coordinates, derived in Červený (2001, eq. 4.14.66). The wavefront orthonormal coordinate system is a local Cartesian coordinate system, connected with the moving wavefront. In the wavefront orthonormal coordinate system y_1, y_2, y_3, coordinates y_1, y_2 are Cartesian coordinates in the plane tangent to the wavefront, with the origin on the reference ray Ω, analogous to ray-centered coordinates q_1, q_2. Coordinate y_3, however, is different from q_3. At any point of the ray, y_3 is chosen along slowness vector $\mathbf{p}$ (perpendicular to the wavefront), not along the ray. Thus, the ray is not a coordinate axis of the wavefront orthonormal coordinate system, and the 6×6 ray propagator matrix in the wavefront orthonormal coordinate system cannot be constructed. However, we can expect that the 4×4 ray propagator matrices in both coordinate systems are the same, as the ray-centered coordinates q_1, q_2 and the wavefront orthonormal coordinates y_1, y_2 coincide at any point of the reference ray Ω. Analogously, we can expect that the 4×4 interface propagator matrices in both coordinate systems are the same. In Červený (2001), the 4×4 interface propagator matrix in wavefront orthonormal coordinates was derived directly, based on the phase matching argument, without invoking the 6×6 interface propagator matrix at all. In the derivation, it was assumed that basis vectors $\mathbf{g}_1$ and $\mathbf{g}_2$ and $\mathbf{n}^\Sigma$ are mutually perpendicular and unit. A 2×2 anisotropy matrix $\boldsymbol{A}^{an}$ was artificially introduced there to transform certain "isotropic" quantities to anisotropic ones. In spite of these differences, it is possible to show that for mutually perpendicular unit vectors $\mathbf{g}_1$ and $\mathbf{g}_2$ both 4×4 interface propagator matrices are fully equivalent, although derived in a quite different way and corresponding to two different coordinate systems. The equation (91) for the 4×4 interface propagator matrix in ray-centered coordinate system, derived here, is however more general, as it allows to construct simply the relevant 6×6 interface propagator matrix (89) from it, and as it uses more general coordinate systems at surfaces. It is also more transparent, as it is expressed in terms of scalar products of basis vectors, and removes fully the artificial anisotropy matrix $\boldsymbol{A}^{an}$. Finally, it is simpler as it uses simpler expressions for the 2×2 matrices $\boldsymbol{E}$ and $\tilde{\boldsymbol{E}}$.

7 Surface-to-surface paraxial matrices in ray-centered coordinates

The 4×4 interface propagator matrix $\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma)$ in ray-centered coordinates, given by (91), can be simply factorized at interface Σ. We introduce the 4×4 matrix $\boldsymbol{Y}$, related to the point of incidence of the reference ray Ω on Σ, and the 4×4 matrix $\tilde{\boldsymbol{Y}}^{-1}$, related to the corresponding reflection/transmission point:

$$\boldsymbol{Y} = \begin{pmatrix} \boldsymbol{K}^{-T} & \boldsymbol{0} \\ (\boldsymbol{E} - \sigma \boldsymbol{D})\boldsymbol{K}^{-1} & \boldsymbol{K} \end{pmatrix}, \qquad \tilde{\boldsymbol{Y}}^{-1} = \begin{pmatrix} \tilde{\boldsymbol{K}}^{T} & \boldsymbol{0} \\ -\tilde{\boldsymbol{K}}^{-1}(\tilde{\boldsymbol{E}} - \tilde{\sigma}\boldsymbol{D}) & \tilde{\boldsymbol{K}}^{-1} \end{pmatrix}. \tag{93}$$

The individual 2×2 matrices in (93) have the same meaning as in (91), see (84), (85) and (86). It is easy to verify that both $\boldsymbol{Y}$ and $\tilde{\boldsymbol{Y}}$ are symplectic. Taking into account that $\mathbf{g}_I = \tilde{\mathbf{g}}_I$ and $\mathbf{g}_{IJ} = \tilde{\mathbf{g}}_{IJ}$ in both matrices $\boldsymbol{Y}$ and $\tilde{\boldsymbol{Y}}^{-1}$, we obtain

$$\boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma) = \tilde{\boldsymbol{Y}}^{-1} \boldsymbol{Y} . \tag{94}$$

Let us briefly discuss the physical meaning of the 4×4 matrix $\boldsymbol{Y}$, related to the point of incidence τ_Σ. It represents the transformation matrix

$$\begin{pmatrix} \delta\boldsymbol{u} \\ \delta\boldsymbol{p}^{(u)} \end{pmatrix} = \boldsymbol{Y} \begin{pmatrix} \delta\boldsymbol{q} \\ \delta\boldsymbol{p}^{(q)} \end{pmatrix} . \tag{95}$$

The meaning of the 2×1 ray-centered vectors $\delta\boldsymbol{q} \equiv (\delta q_1, \delta q_2)^T$ and $\delta\boldsymbol{p}^{(q)} \equiv (\delta p_1^{(q)}, \delta p_2^{(q)})^T$ is explained in detail under Equation (48). Relation (95) transforms vectors $\delta\boldsymbol{q}$ and $\delta\boldsymbol{p}^{(q)}$ (measured along the plane tangent to the wavefront) into $\delta\boldsymbol{u} \equiv (\delta u_1, \delta u_2)^T$ and $\delta\boldsymbol{p}^{(u)} \equiv (\delta p_1^{(u)}, \delta p_2^{(u)})^T$, measured along surface Σ. Vector $\delta\boldsymbol{u}$ determines the position of the point of incidence of the paraxial ray under consideration on surface Σ. Vector $\delta\boldsymbol{p}^{(u)} \equiv (\delta p_1^{(u)}, \delta p_2^{(u)})^T$ represents the difference between the tangential components of the slowness vector at the point of incidence of the paraxial ray and at the point of incidence of reference ray Ω.

At the point of reflection/transmission of the reference ray Ω at Σ, matrix $\tilde{\boldsymbol{Y}}$ has a meaning analogous to (95):

$$\begin{pmatrix} \delta\tilde{\boldsymbol{q}} \\ \delta\tilde{\boldsymbol{p}}^{(q)} \end{pmatrix} = \tilde{\boldsymbol{Y}}^{-1} \begin{pmatrix} \delta\boldsymbol{u} \\ \delta\boldsymbol{p}^{(u)} \end{pmatrix} . \tag{96}$$

As the tangential components of the slowness vector are continuous across Σ (Snell's law), $\delta\boldsymbol{u}$ and $\delta\boldsymbol{p}^{(u)}$ should be the same on both sides of Σ. Combining (95) with (96), we get:

$$\begin{pmatrix} \delta\tilde{\boldsymbol{q}} \\ \delta\tilde{\boldsymbol{p}}^{(q)} \end{pmatrix} = \tilde{\boldsymbol{Y}}^{-1}\boldsymbol{Y} \begin{pmatrix} \delta\boldsymbol{q} \\ \delta\boldsymbol{p}^{(q)} \end{pmatrix} = \boldsymbol{\Pi}^{(q)}(\tilde{\tau}_\Sigma, \tau_\Sigma) \begin{pmatrix} \delta\boldsymbol{q} \\ \delta\boldsymbol{p}^{(q)} \end{pmatrix} . \tag{97}$$

This corresponds fully to the definition of the 4×4 interface propagator matrix in ray-centered coordinates, see (94).

Consider now the reference ray Ω, with the initial point at S and end point at R, incident at surface Σ at point Q, with the relevant reflection/transmission point $\tilde{Q}$. The chain rule in ray-centered coordinates reads:

$$\boldsymbol{\Pi}^{(q)}(R,S) = \boldsymbol{\Pi}^{(q)}(R,\tilde{Q})\boldsymbol{\Pi}^{(q)}(\tilde{Q},Q)\boldsymbol{\Pi}^{(q)}(Q,S) . \tag{98}$$

Using (94), we can replace the 4×4 interface propagator matrix $\boldsymbol{\Pi}^{(q)}(\tilde{Q},Q)$ by $\boldsymbol{Y}^{-1}(\tilde{Q})\,\boldsymbol{Y}(Q)$. Consider further that the point S is situated on the anterior surface Σ^a and point R on the posterior surface Σ^p. Multiplying (98) by $\boldsymbol{Y}(R)$ from the left and by $\tilde{\boldsymbol{Y}}^{-1}(S)$ from the right, we obtain

$$\boldsymbol{Y}(R)\boldsymbol{\Pi}^{(q)}(R,S)\,\tilde{\boldsymbol{Y}}^{-1}(S) = \boldsymbol{Y}(R)\boldsymbol{\Pi}^{(q)}(R,\tilde{Q})\,\tilde{\boldsymbol{Y}}^{-1}(\tilde{Q})\,\boldsymbol{Y}(Q)\boldsymbol{\Pi}^{(q)}(Q,S)\,\tilde{\boldsymbol{Y}}^{-1}(S) .$$

We now introduce the 4×4 surface-to-surface paraxial matrix $\boldsymbol{T}(R,S)$ in ray-centered coordinates by the relation

$$\boldsymbol{T}(R,S) = \boldsymbol{Y}(R)\boldsymbol{\Pi}^{(q)}(R,S)\,\tilde{\boldsymbol{Y}}^{-1}(S) . \tag{99}$$

The above equation then yields

$$\boldsymbol{T}(R,S) = \boldsymbol{T}(R,\tilde{Q})\,\boldsymbol{T}(Q,S) . \tag{100}$$

The requirement is that Q corresponds to the point of incidence of the reference ray Ω on surface Σ and $\tilde{Q}$ to the relevant reflection/transmission point on the same surface Σ, so that $\mathbf{g}_I(Q)$ and $\mathbf{g}_{IJ}(Q)$ are the same as $\mathbf{g}_I(\tilde{Q})$ and $\mathbf{g}_{IJ}(\tilde{Q})$. The 2×2 surface-to-surface paraxial matrix $\boldsymbol{T}(R,S)$ satisfies the symplectic property, its determinant equals unity, and may be further chained. If the ray crosses n interfaces $\Sigma_1, \Sigma_2, ..., \Sigma_n$ between S and R,

$$\boldsymbol{T}(R,S) = \boldsymbol{T}(R,\tilde{Q}_n)\,\boldsymbol{T}(Q_n,\tilde{Q}_{n-1})...\boldsymbol{T}(Q_2,\tilde{Q}_1)\,\boldsymbol{T}(Q_1,S)\ . \tag{101}$$

The continuation relation reads:

$$\begin{pmatrix} \delta\boldsymbol{u}(R) \\ \delta\boldsymbol{p}^{(u)}(R) \end{pmatrix} = \boldsymbol{T}(R,S) \begin{pmatrix} \delta\boldsymbol{u}(S) \\ \delta\boldsymbol{p}^{(u)}(S) \end{pmatrix}\ . \tag{102}$$

Consequently, the surface-to-surface paraxial matrix transforms the paraxial ray quantities $\delta\boldsymbol{u}$ and $\delta\boldsymbol{p}^{(u)}$ from one surface to another. The surfaces may be of an arbitrary shape and may represent geological interfaces, the surface of the Earth, isochrone surfaces, or merely formal surfaces. The formal surfaces can be introduced at any point of the reference ray. It is, however, required that the physical surfaces (structural interfaces) do not intersect in the paraxial vicinity of the reference ray.

The surface-to-surface paraxial matrices are closely linked to the so-called theory of seismic systems. For a medium composed of homogeneous and inhomogeneous isotropic layers, see Bortfeld (1989), Hubral et al. (1992,1993,1995), Schleicher et al. (1993), Červený (2001, sec. 4.4.7), Chira-Oliva et al. (2001), Biloti et al. (2002), Sun (2004). For anisotropic structures, a most detailed treatment, with many applications and references, can be found in Moser and Červený (2006). The derivations in the last reference are based on the factorization of the interface propagator matrix expressed in Cartesian coordinates. Analogously, the factorization of the interface propagator matrix in wavefront orthonormal coordinates was used by Červený (2001, sec. 4.14.10) to derive the surface-to-surface paraxial matrices in these coordinates. See also Section 6 for comparison of the interface propagator matrix in wavefront-orthonormal and ray-centered coordinates. Similarly as the interface propagator matrices, the surface-to-surface paraxial matrices in wavefront orthonormal coordinates can be obtained as a special case of the equations derived here.

A terminological note: The surface-to-surface paraxial matrix has also been referred to as the surface-to-surface propagator matrix in the seismological literature. This term was used to emphasize that the paraxial solutions $\delta\boldsymbol{u}$ and $\delta\boldsymbol{p}^{(u)}$ can be "propagated" from one surface to another, see (102). Mathematically, however, the surface-to-surface paraxial matrices are not propagator matrices, see Gilbert and Backus (1966), Ursin (1983). To avoid possible confusion, we use the term surface-to-surface paraxial matrices consistently. Analogous terminology was also used by Moser and Červený (2006).

The formalism of surface-to-surface paraxial matrices offers many useful applications of both theoretical and practical interest. Certain of these applications are discussed in detail by Moser and Červený (2006), where also appropriate references can be found. See also the next section.

8 Concluding remarks

We have proposed two methods of calculating the 4×4 ray propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates along the reference ray Ω from τ_0 to τ. None of these methods requires dynamic ray tracing in ray-centered coordinates; both are based fully on conventional dynamic ray tracing in Cartesian coordinates.

1) In the first method, $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ is computed from the 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates, using (62) with (63).

2) In the second method, $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ is computed using (71). This method does not require the whole 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates to be known, but only four solutions of the dynamic ray tracing system in Cartesian coordinates, for strictly specified initial conditions (72).

Both methods should yield the same 4×4 ray propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates; the differences are only in the numerical efficiency of the computations. The second method is in general numerically more efficient than the first method, as it avoids the unnecessary computation of elements in the third and sixth columns and rows of $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$, which are later removed.

In some exceptional cases, the first method may be more useful than the second. This applies to the case in which we need to know $\boldsymbol{\Pi}^{(q)}(\tau, \tau_0)$ for various initial conditions. In this case, it may be useful to compute the whole 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$, and vary only $\mathbf{\Psi}_2^r(\tau_0)$. We do not need to perform new dynamic ray tracing in Cartesian coordinates when we change the matrix of initial conditions $\mathbf{\Psi}_2^r(\tau_0)$.

Analogously to the two methods to determine 4×4 propagator matrices $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates described above, we can also compute the 6×6 ray-propagator matrix $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ in ray-centered coordinates. In the first method, we use (61) with (59), and in the second method (64).

Let us now consider any point Q situated on the reference ray Ω between τ_0 and τ. Assuming the 6×6 propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ is known along the ray from τ_0 to τ, including the point τ_Q, we can evaluate the 4×4 propagator matrix $\boldsymbol{\Pi}^{(q)}(\tau_Q, \tau_0)$ at that point using (62), where we replace τ by τ_Q. Analogously, we can store $\mathbf{Z}^r(\tau_Q, \tau_0)$ and use (71), where we again replace τ by τ_Q. Actually, the only additional work is the computation of the 4×6 matrix $\mathbf{\Psi}_1^r(\tau_Q)$ at point Q.

A note to the choice of basis vectors $\mathbf{e}_I(\tau_0)$, $\mathbf{e}_I(\tau)$, $\mathbf{f}_I(\tau_0)$ and $\mathbf{f}_I(\tau)$. Assume first that $\mathbf{e}_I(\tau_0)$ are chosen as mutually perpendicular unit vectors, perpendicular to the slowness vector $\mathbf{p}(\tau_0)$. Actually, it is sufficient to specify only $\mathbf{e}_1(\tau_0)$, as $\mathbf{e}_2(\tau_0) = \mathcal{C}(\tau_0)\mathbf{p}(\tau_0) \times \mathbf{e}_1(\tau_0)$. The orientation of unit vector $\mathbf{e}_1(\tau_0)$ (perpendicular to $\mathbf{p}(\tau_0)$), however, may be quite arbitrary in the plane perpendicular to slowness vector $\mathbf{p}(\tau_0)$. Vectors $\mathbf{f}_I(\tau_0)$ must, of course, strictly correspond to this choice of $\mathbf{e}_I(\tau_0)$, see (31). The same is valid even at point τ: We can choose $\mathbf{e}_I(\tau)$ arbitrarily.

Analogous rules are valid even if we choose $\mathbf{f}_I(\tau_0)$ as mutually perpendicular unit vectors, perpendicular to the ray velocity vector $\boldsymbol{\mathcal{U}}(\tau_0)$. It is again sufficient to specify unit vector $\mathbf{f}_1(\tau_0)$ arbitrarily in the plane perpendicular to $\boldsymbol{\mathcal{U}}(\tau_0)$; vector $\mathbf{f}_2(\tau_0) = (\boldsymbol{\mathcal{U}}(\tau_0) \times \mathbf{f}_1(\tau_0))/\mathcal{U}(\tau_0)$. Vectors $\mathbf{e}_I(\tau_0)$, however, must strictly correspond to the choice of $\mathbf{f}_I(\tau_0)$, see (32). The same is again valid at point τ: We can choose $\mathbf{f}_I(\tau)$ arbitrarily.

A final remark. In Section 6, the expressions for the 6×6 interface propagator matrix in ray-centered coordinates were derived from the expression for the 6×6 interface propagator matrix in Cartesian coordinates, given by Moser (2004). It is shown how this expression is reduced from 6×6 to 4×4 interface propagator matrix. This extends the possibilities of dynamic ray tracing in ray-centered coordinates also to anisotropic inhomogeneous media with structural interfaces. In Section 7, the expression for interface propagator matrix is factorized and used to derive the 4×4 surface-to-surface paraxial matrices in ray-centered coordinates. Such 4×4 surface-to-surface paraxial matrices offer many important applications in the paraxial ray methods for inhomogeneous anisotropic layered media. To keep the paper to an admissible length, we do not discuss these applications here; we only briefly list several of them: a) Solution of boundary-value ray tracing problems in four-parameteric system of paraxial rays connecting two surfaces. b) Determination of the slowness vectors at initial and end points of a paraxial ray connecting two surfaces. c) Two-point eikonal, i.e. the travel time along a paraxial ray connecting any point of one surface with any point of other surface. d) Determination of relative geometrical spreading, needed in the computation of the ray-theory Green's function. e) Determination of relative geometrical spreading from the travel time measurements along the two surfaces. f) Determination of the complete ray propagator matrix from the mixed second derivatives of the travel time field along two surfaces. g) Determination of the Fresnel zone matrix and Fresnel regions. h) Factorization of relative geometrical spreading using the Fresnel zone matrix. i) Isochrons. Isochron rays. j) Point to curve ray tracing. k) Computation of Gaussian beams and Gaussian beams and Gaussian packets. l) Computation of Maslov synthetic seismograms. m) Application in ray-perturbation theory. n) Application in various diffraction problems. Edge and tip waves. o) Applications in the true-amplitude migration and in the theory of Kirchhoff-Helmholtz integrals. For more details, we refer the reader to Hubral et al. (1992, 1993), Farra (1999), Červený (2001, Chap. 4), Hanyga et al. (2001), Gjøystdal et al. (2002), Chapman (2004), Iversen (2004b), Sun (2004), Moser and Červený (2006), where many other references can be found. Of course, the surface-to-surface paraxial matrices in ray-centered coordinates are primarily suitable for implementation into ray tracing packages, based on ray-centered coordinates.

Acknowledgements

The authors are greatly indebted to Chris Chapman, Luděk Klimeš and Ivan Pšenčík for helpful suggestions and valuable discussions. This research has been supported by the Grant Agency of the Czech Republic under the Contracts 205/01/D097 and 205/04/1104, and by the Consortium "Seismic Waves in Complex 3-D Structures". Part of this work has been done during TJM's stays at the Charles University, Prague, sponsored by the EC project EVG3-CT-2002-80006 (MAGMA).

References

Bakker, P.M. , 1996. Theory of anisotropic dynamic ray tracing in ray-centered coordinates. *PAGEOPH*, **148**, 583 - 589.

Biloti, R., Santos, L.T., and Tygel, M., 2002. Multiparametric traveltime inversion. *Stud. Geoph. Geod.*, **46**, 177 -192.

Bortfeld, R., 1989. Geometric ray theory: Rays and traveltimes in seismic systems (second-order approximation of the traveltimes). *Geophysics*, **54**, 342 - 349.

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

Červený, V., 2001. *Seismic ray theory.* Cambridge: Cambridge Univ. Press.

Červený, V., and Hron, F., 1980. The ray series method and dynamic ray tracing system for three-dimensional inhomogeneous media. *Bull. Seismol. Soc. Am.*, **70**, 47 - 77.

Červený, V., Klimeš, L., and Pšenčík, I., 1988. Complete seismic ray tracing in three-dimensional structures. In: *Seismological algorithms*, ed. D. J. Doornbos, pp. 89 - 168. New York : Academic Press.

Červený, V., Langer, J., and Pšenčík, I., 1974. Computation of geometrical spreading of seismic body waves in laterally inhomogeneous media with curved interfaces. *Geophys. J.R. astr. Soc.*, **38**, 9 - 19.

Chapman, C. H., 2004. *Fundamentals of seismic wave propagation.* Cambridge: Cambridge Univ. Press.

Chira-Oliva, P., Tygel, M., Zhang, Y., and Hubral, P., 2001. Analytic CRS formula for a 2D curved measurement surface and finite-offset reflections. *J. Seis. Exploration*, **10**, 245 - 262.

Farra, V., 1989. Ray perturbation theory for heterogeneous hexagonal anisotropic medium. *Geophys. J. Int.*, **99**, 723 - 738.

Farra, V., and LeBégat, S., 1995. Sensitivity of qP wave traveltimes and polarization vectors to heterogeneity, anisotropy and interfaces. *Geophys. J. Int.*, **121**, 371 - 384.

Gajewski, D., and Pšenčík, I., 1987. Computation of high-frequency seismic wavefields in 3-D laterally inhomogeneous anisotropic media. *Geophys. J. R. astr. Soc.*, **91**, 383 - 411.

Gajewski, D., and Pšenčík, I., 1990. Vertical seismic profile synthetics by dynamic ray tracing in laterally varying layered anisotropic structures. *J. Geophys. Res.*, **95**, 11301 - 11315.

Gilbert, F., and Backus, G.E., 1966. Propagator matrices in elastic wave and vibration problems. *Geophysics*, **31**, 326 - 332.

Gjøystdal, H., Iversen, E., Laurain, R., Lecomte, I., Vinje, V., and Åstebol, K, 2002.

Review of ray theory applications in modelling and imaging of seismic data. *Stud. Geoph. Geod.*, **46**, 113 - 164.

Hanyga, A., 1982. Dynamic ray tracing in anisotropic medium. *Tectonophysics*, **90**, 243 - 251.

Hanyga, A., Druzhinin, A. B., Dzhafarov, A. D., Frøyland, L., 2001. A Hamiltonian approach to asymptotic seismic reflection and diffraction modeling. *Geoph. Prosp.*, **49**, 213 - 227.

Hubral, P., Schleicher, J., and Tygel, M., 1992. Three-dimensional paraxial ray properties: Part I. Basic relations. *J. Seis. Exploration*, **1**, 265 - 279. Part II. Applications. *J. Seis. Exploration*, **1**, 347 - 362.

Hubral, P., Schleicher, J., and Tygel, M., and Hanitzsch, C., 1993. Determination of Fresnel zones from traveltime measurements. *Geophysics*, **58**, 703 - 712.

Hubral, P., Tygel, M., and Schleicher, J., 1995. Geometrical spreading and ray-caustics decomposition of elementary seismic waves. *Geophysics*, **60**, 1195 - 1202.

Iversen, E., 2004a. Reformulated kinematic and dynamic ray tracing systems for arbitrary anisotropic media. *Stud. Geoph. Geod.*, **48**, 1-20.

Iversen, E., 2004b. The isochron ray in seismic modeling and imaging. *Geophysics*, **69**, 1053 - 1070.

Kendall, J-M., Guest, W., S., and Thomson, C. J., 1992. Ray theory Green's function reciprocity and ray-centered coordinates in anisotropic media. *Geophys. J. Int.*, **108**, 364 - 371.

Kennett, B.L.N., 1983. *Seismic wave propagation in stratified media.* Cambridge: Cambridge Univ. Press.

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

Klimeš, L., 2006. Ray-centered coordinate systems in anisotropic media. *Stud. Geoph. Geod.,*, **50**, in press.

Moser, T.J., 2004. Review of the anisotropic interface ray propagator: symplecticity, eigenvalues, invariants and applications. *Stud. Geoph. Geod.*, **48**, 47 - 73.

Moser, T.J., and Červený, V., 2006. Paraxial ray methods for anisotropic inhomogeneous media. *Geophys. Prospecting*, in press.

Norris, A. N., 1987. A theory of pulse propagation in anisotropic elastic solids. *Wave Motion*, **9**, 509 - 532.

Popov, M. M., and Pšenčík, I., 1978a. Ray amplitudes in inhomogeneous media with curved interfaces. In *Geofyzikální sborník*, vol. 24, ed. A Zátopek, pp.111 - 129. Praha: Academia.

Popov, M. M., and Pšenčík, I., 1978b. Computation of ray amplitudes in inhomogeneous media with curved interfaces. *Stud. Geoph. Geod.*, **22**, 248 - 258.

Pšenčík, I., and Teles, T. N., 1996. Point source radiation in inhomogeneous anisotropic structures. *PAGEOPH*, **148**, 591 - 623.

Sun, J., 2004. True amplitude weight function in 3D limited aperture migration revisited. *Geophysics*, **60**, 1025 - 1036.

Shearer, P. M., and Chapman, C. H., 1989. Ray tracing in azimuthally anisotropic media. I. Results for models of aligned cracks in the upper crust. *Geophys. J.*, **96**, 51 - 64.

Schleicher, J., Tygel, M., and Hubral, P., 1993. 3-D true-amplitude finite-offset migration. *Geophysics*, **58**, 1112 - 1126.

Ursin, B., 1983. Review of elastic and electromagnetic wave propagation in horizontally layered media. *Geophysics*, **48**, 1063 - 1081.