Gaussian beams in inhomogeneous anisotropic layered structures

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Summary

Gaussian beams concentrated close to rays of high-frequency seismic body waves propagating in an inhomogeneous anisotropic layered structure are studied. The amplitude profiles of the Gaussian beam along the plane perpendicular to the ray and along the plane perpendicular to the slowness vector are Gaussian. The Gaussian profile is controlled by the 2×2 complex-valued matrix $\mathbf{M}$ of the second derivatives of the travel-time field at any point of the ray. The matrix $\mathbf{M}$ can be simply determined at any point of the ray if the ray-propagator matrix along the ray is known and if the value of $\mathbf{M}$ is specified at a selected point of the ray. The ray-propagator matrix can be determined by dynamic ray tracing along the ray. In inhomogeneous anisotropic medium, the dynamic ray tracing can be performed alternatively in several coordinate systems: in global Cartesian coordinates, in ray-centred coordinates and in wavefront orthonormal coordinates. In addition, also simplified dynamic ray tracing in global Cartesian coordinates can be used, which reduces the number of equations of the dynamic ray tracing system. The derived expressions for the Gaussian beams are applicable to general 3-D inhomogeneous layered structures of arbitrary anisotropy (specified by upto 21 independent position-dependent elastic moduli). Possible simplification of the procedure are outlined.

Keywords: Paraxial travel times, Gaussian beams, dynamic ray tracing, anisotropic heterogeneous medium.

1 Introduction

The method of summation of Gaussian beams is a powerful extension of the ray method. It is based on the summation of Gaussian beams concentrated close to rays traced from the source or from an initial surface. The amplitudes of Gaussian beams decrease exponentially with the square of the distance from the central ray in the plane tangent

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to the wavefront and in the plane perpendicular to the ray. The amplitude profiles in these planes are Gaussian. This is the reason why these beams are called Gaussian beams. The final equations for Gaussian beams are valid along the whole central ray and Gaussian beams have a singularity neither at caustics nor at any other point of the ray.

The Gaussian beams discussed here are not exact solutions of the elastodynamic equation. In a vicinity of the central ray, called paraxial vicinity, the complex-valued travel time of the beam is approximated by its quadratic expansion. To distinguish these beams from exact Gaussian beams, which satisfy the elastodynamic equation exactly, we often call them the paraxial Gaussian beams. In seismological literature, however, it is common to call them Gaussian beams, without emphasizing their approximate validity in the paraxial vicinity of the central ray. In this paper, we call them simply "Gaussian beams", without emphasizing the paraxial validity of their equations.

The theory of Gaussian beams in isotropic heterogeneous layered structures has been described in many papers published in seismological journals. For scalar wave equation, see Babich (1968), Babich and Popov (1981), Popov (1982), Červený, Popov and Pšenčík (1982). For elastodynamic isotropic wave equation, see Červený and Pšenčík (1983a,b), Klimeš (1984), Červený (1985), George et al. (1987), White, Norris, Bayliss and Burridge (1987), Popov (2002), Bleistein (2007), Červený, Klimeš and Pšenčík (2007), Kravtsov and Berczynski (2007), Leung, Qian and Burridge (2007). Gaussian beam summation method has been successfully applied in migration in seismic exploration. A description of the theory of Gaussian beam migration, of its algorithm and excellent results can be found in Hill (1990, 2001), Gray (2005), Vinje, Roberts and Taylor (2008), Gray and Bleistein (2009). The references to the theory and applications of Gaussian beams propagating in inhomogeneous anisotropic media are not so common. We have to refer to an excellent mathematical treatment by Ralston (1983), devoted to Gaussian beams and propagation of singularities, and to Hanyga (1986). In seismic migration for anisotropic media, the Gaussian beam method was applied by Alkhalifah (1995).

As the problem of summation of Gaussian beams in heterogeneous anisotropic layered media is more involved and may be discussed from several aspects, we concentrate here on study of individual Gaussian beams only, not on the summation integrals. We plan to concentrate on the problem of Gaussian beam summation in future. Here we try to derive and explain several alternative approaches to determine Gaussian beams. Some of these approaches may be more efficient than others. The problem of the numerical efficiency of proposed algorithms requires a further investigation. The most time consuming step in the computation of Gaussian beams consists in ray tracing of their central rays, and, partially, in dynamic ray tracing along these rays. The methods of ray tracing are well known and are discussed only briefly in this paper. We only emphasize that ray tracing in inhomogeneous anisotropic media is considerably more time consuming than in isotropic media. The dynamic ray tracing consists in the solution of several linear ordinary differential equations (DRT system) of the first order along the central ray. The dynamic ray tracing is a procedure which can be used to obtain approximate variation of certain quantities, obtained from ray tracing just along the central ray, also in the paraxial vicinity of this ray. The most important of these quantities is the paraxial travel time. The dynamic ray tracing can be performed in several coordinate systems, e.g., in global Cartesian coordinates, in ray-centred coordinates (in which the central ray is one of the coordinate axes of the system), etc. In global Cartesian coordinates, the DRT system consists of six equations, in ray-centred coordinates of four equations. The DRT system must usually be solved several times, with different initial conditions, depending on the purpose of computations. Dynamic ray tracing can be also used to to determine very useful propagator matrix, which can be used in many important applications, including the computation of Gaussian beams and their summation.

To express the equations of the paper in a concise form, we use alternatively the component and matrix notation for vectors and matrices. In the component notation, the upper-case indices (I, J, K,...) take the values 1 or 2, and the lower-case indices (i, j, k,...) the values 1, 2, or 3. Einstein summation convention is used throughout the paper. The matrices and vectors are denoted by bold upright symbols. The vectors are considered as column matrices. In this way, scalar product of vectors $\mathbf{a}$ and $\mathbf{b}$ reads $\mathbf{a}^T\mathbf{b}$, dyadic reads $\mathbf{a}\mathbf{b}^T$. To distinguish the 2×2 matrices from 3×3 matrices, the 3×3 matrices are denoted by the circumflex above the letter. Whenever there may be reason for confusion, the dimensions of the matrices are explicitly indicated. Some quantities depend on the coordinate system (Cartesian coordinates x_i, tay-centred coordinates q_i, etc.), in which they are specified. In certain parts of the paper, we use, therefore, quantities with superscripts (x), (q), etc., in order to emphasize which coordinate system is used. See, for example, equation (43) for the relation between $\hat{\mathbf{M}}^{(x)}$ and $\mathbf{M}^{(q)}$.

The Gaussian beams represent an extension of the ray concepts. For this reason, it is useful to introduce briefly some of these concepts in the following.

Let us consider a heterogeneous anisotropic perfectly elastic medium. The source-free elastodynamic equation for this medium reads:

$$(c_{ijkl}u_{k,l})_{,j} = \rho\, \ddot{u}_i \ . \tag{1}$$

Here $u_i(x_n)$ are the Cartesian components of the displacement vector $\mathbf{u}(x_n)$, $c_{ijkl}(x_n)$ are real-valued elastic moduli, and $\rho(x_n)$ the density. In the zero-order approximation of the ray method, the time-harmonic solution of (1) for any high-frequency seismic body wave is usually expressed in the following form:

$$\mathbf{u}(x_i, t) = \mathbf{U}(x_i) \exp[-\mathrm{i}\omega(t - T(x_j))] \ . \tag{2}$$

Here $T(x_i)$ is the travel time, $\mathbf{U}(x_i)$ the complex-valued vectorial amplitude, ω the circular frequency, t time and x_i the Cartesian coordinates. Inserting (2) into (1), we obtain the system of three equations

$$(\Gamma_{ik} - \delta_{ik})U_k = 0 \ , \qquad i = 1, 2, 3 \ . \tag{3}$$

The 3×3 matrix $\mathbf{\Gamma}(x_m, p_n)$ is given by the relation

$$\Gamma_{ik}(x_m, p_n) = a_{ijkl}p_j p_l \ , \tag{4}$$

and is usually called the generalized Christoffel matrix. Here a_{ijkl} are the density-normalized elastic moduli

$$a_{ijkl}(x_n) = c_{ijkl}(x_n)/\rho(x_n) \ . \tag{5}$$

The quantities $p_i = \partial T/\partial x_i$ are Cartesian components of the slowness vector $\mathbf{p}$.

The Christoffel matrix (4) has three eigenvalues $G_m(x_n, p_m)$ and three relevant eigenvectors $\mathbf{g}^{(m)}(x_n, p_m)$, $m = 1, 2, 3$. They correspond to the three relevant elementary waves, propagating in heterogeneous anisotropic media, namely P, S1 and S2. Since matrix $\mathbf{\Gamma}$ is symmetric and positive definite, all the three eigenvalues G_1, G_2 and G_3 are real-valued and positive. Moreover, they are homogeneous functions of second degree in p_i. For simplicity, we consider in the following that all three eigenvalues are different.

Let us consider the m-th elementary wave. It follows from (3) that the eigenvalue G_m of this wave satisfies the relation

$$G_m(x_n, p_m) = 1 \ . \tag{6}$$

Equation (6) is a non-linear partial differential equation of the first order for the travel time function $T(x_i)$. It is usually called the eikonal equation for heterogeneous anisotropic medium. It can be expressed in the Hamiltonian form

$$\mathcal{H}(x_i, p_j) = \tfrac{1}{2}(G_m(x_i, p_j) - 1) = 0 \ . \tag{7}$$

The Hamiltonian function $\mathcal{H}(x_i, p_j)$ is used in the ray tracing, see Appendix A, from which the travel time is usually computed.

The vectorial amplitude $\mathbf{U}$ can be expressed in terms of the unit real-valued eigenvector $\mathbf{g}^{(m)}$ of the Christoffel matrix (4) as follows:

$$\mathbf{U}(x_i) = A(x_i)\mathbf{g}^{(m)}(x_i) \ . \tag{8}$$

Here $A(x_i)$ is a complex-valued frequency-independent scalar amplitude. See Section 2.3. Equation (8) shows that the eigenvector $\mathbf{g}^{(m)}$ specifies the polarisation of the wave under consideration. For this reason, we call $\mathbf{g}^{(m)}(x_i)$ the polarisation vector.

2 Ray tracing, dynamic ray tracing and ray-theory amplitudes in inhomogeneous anisotropic layered structures

In this section, we discuss basic techniques of computing ray-theory quantities of an arbitrary high-frequency seismic body wave propagating in an inhomogeneous anisotropic layered structure. In Sec.4, we generalize these techniques for the computation of Gaussian beams.

2.1 Ray tracing

Let us consider an arbitrary high-frequency seismic body wave (P, S1, S2; direct, reflected, transmitted, multiply reflected/transmitted, etc.) propagating in an inhomogeneous anisotropic layered structure. We can use *ray tracing* to compute any ray Ω of the two-parametric (orthonomic) system of rays corresponding to a selected wave, and denote its ray parameters γ_1 and γ_2. Ray tracing system consists of generally nonlinear ordinary differential equations of the first order. We can introduce a monotonically increasing sampling parameter γ_3 along the ray Ω, which uniquely specifies the position of a point on the ray Ω. The sampling parameter γ_3 may be chosen in different ways. In inhomogeneous anisotropic media, it is most convenient to take $\gamma_3 = \tau$, where τ is the travel time T along the ray Ω of the wave under consideration. Ray tracing equations for inhomogeneous anisotropic media are given in Appendix A. Appendix A also presents the transformation equations of the ray at a structural interface.

From ray tracing, we obtain coordinates $\mathbf{x}(\tau)$ of points along the ray trajectory Ω and slowness vectors $\mathbf{p}(\tau)$ at these points. As a by-product of ray tracing, we can determine several other useful quantities, which we shall need in the following: the ray-velocity vector $\boldsymbol{\mathcal{U}}(\tau) = d\mathbf{x}(\tau)/d\tau$, the unit vector $\mathbf{t}(\tau) = \boldsymbol{\mathcal{U}}(\tau)/|\boldsymbol{\mathcal{U}}(\tau)|$ tangent to the ray Ω, the unit vector $\mathbf{N}(\tau) = \mathbf{p}(\tau)/|\mathbf{p}(\tau)|$ perpendicular to the wavefront, the vector $\boldsymbol{\eta}(\tau) = d\mathbf{p}(\tau)/d\tau$, which represents the variations of the slowness vector along the ray, the polarization vector $\mathbf{g}(\tau)$, the phase velocity $\mathcal{C}(\tau) = 1/|\mathbf{p}(\tau)|$, the ray velocity $\mathcal{U} = |\boldsymbol{\mathcal{U}}(\tau)|$. The ray-velocity vector is also sometimes called the energy-velocity vector or the group-velocity vector. In non-dissipative media, all these terms have the same meaning. The travel time along the ray $T(\tau)$ is automatically determined as it equals the sampling parameter along the ray, $T(\tau) = \tau$. In the following, we consider the so-called initial-valued rays specified by the initial conditions $\tau = \tau_0$, $\mathbf{x}(\tau_0) = \mathbf{x}_0$, $\mathbf{p}(\tau_0) = \mathbf{p}_0$, where τ_0 is an arbitrarily chosen initial time.

In certain applications, it may be useful to take a different sampling parameter along the ray Ω than τ. In seismic exploration, it is common to consider one Cartesian coordinate, particularly the depth, as a sampling parameter. This reduces the number of equations in the ray-tracing system, but does not guarantee that the sampling parameter varies monotonically along the ray. If depth is used as the sampling parameter, the problems occur at the turning points, where the rays change their direction with respect to the depth. Such cases require special attention. If, however, the rays do not have turning points, the Gaussian beams concentrated close to the rays parameterized in this way can be computed without problems. To avoid problems with turning points, we use exclusively the monotonic sampling parameters along rays, specifically $\gamma_3 = \tau$, in the following. The Gaussian beams concentrated to rays with γ_3 equal to depth will be investigated elsewhere.

The ray tracing can be used to compute all the above-mentioned quantities only on the considered ray Ω, not in its vicinity. This is, however, not sufficient for the calculation of ray-theory amplitudes and/or Gaussian beams concentrated to the ray Ω. This is because the ray-theory amplitudes depend on the geometrical spreading, which is a function of the ray field, not of a single ray. In the case of Gaussian beams, we also need to compute paraxial travel times (travel times in a vicinity of the ray Ω). To make computation of quantities related to the ray field possible, it is necessary to supplement the ray tracing by an additional procedure called *dynamic ray tracing.*

2.2 Dynamic ray tracing

Dynamic ray tracing (DRT) consists of a system of linear ordinary differential equations of the first order to be solved along the ray Ω, commonly several times. It can be solved together with the ray tracing system or along an a priori known ray. The DRT system in **global Cartesian coordinates** can be used to compute the following partial derivatives along the ray Ω:

$$Q_{ij} = \partial x_i / \partial \gamma_j \ , \qquad P_{ij} = \partial p_i / \partial \gamma_j \ . \tag{9}$$

The 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ describe changes of the ray trajectory $\mathbf{x}(\tau)$ and of the relevant slowness vector $\mathbf{p}(\tau)$ caused by changes of the ray coordinates γ_1, γ_2 and $\gamma_3 = \tau$. The actual form of the DRT system in global Cartesian coordinates is presented in Appendix B.

In 3D models, the DRT system in global Cartesian coordinates x_i consists of 6 equations for Q_{ij} and P_{ij} specified for one of the ray coordinates γ_j. Consequently, the whole 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ are obtained by solving the DRT system three times, each time with proper initial conditions corresponding to considered γ_j. The system is computationally efficient as it is linear and, except the second-order derivatives of the generalized Christoffel matrix $\mathbf{\Gamma}$, it requires only quantities already calculated during ray tracing. Moreover, the three solutions of the DRT system can be sought together so that the coefficients of the DRT system are evaluated only once.

The DRT is a basic procedure for the computation of the geometrical spreading and, consequently, for the ray quantities as the ray-theory amplitudes, which describe dynamics of waves. Therefore, we speak about dynamic ray tracing in order to distinguish it from the standard ray tracing, which is often called kinematic ray tracing. The DRT can be also used to compute the second partial derivatives of travel time $T = T(x_m)$ with respect to spatial coordinates x_i:

$$M_{ij} = \frac{\partial^2 T(x_m)}{\partial x_i \, \partial x_j} \ . \tag{10}$$

It is easy to show that the 3×3 symmetric matrix $\hat{\mathbf{M}}$ with nine components M_{ij} can be simply expressed in terms of 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ obtained from the dynamic ray tracing and ray tracing. As

$$M_{ij} Q_{jk} = \frac{\partial^2 T}{\partial x_i \, \partial x_j} \frac{\partial x_j}{\partial \gamma_k} = \frac{\partial p_i}{\partial \gamma_k} = P_{ik} \ , \tag{11}$$

we obtain

$$\hat{\mathbf{M}} = \hat{\mathbf{P}} \hat{\mathbf{Q}}^{-1} \ . \tag{12}$$

Actually, the 3×3 matrix $\hat{\mathbf{M}}$ can be also computed directly from the Ricatti equation solved along the ray. The Ricatti equation is, however, nonlinear and thus it is not as suitable for computations as the system of linear dynamic ray tracing equations. Moreover, DRT system can be used to construct ray-propagator matrices, which play an important role in the computation of Gaussian beams. The Ricatti equation cannot be used for this purpose.

The applications of the DRT are much broader than those discussed above. As the travel time $T = \tau$ and its first derivatives $p_i = \partial T / \partial x_i$ are known from kinematic ray tracing and the second derivatives $M_{ij} = \partial^2 T / \partial x_i \, \partial x_j$ can be determined using the DRT at any point of the ray, we can use a quadratic expansion of the travel time at that point and determine, approximately, the distribution of the travel time $T(x_m)$ even in a vicinity of the ray Ω. We speak of paraxial approximation of travel time and of quadratic or paraxial vicinity of the ray. We can also determine linear expansion of the slowness vector and compute paraxial rays in the paraxial vicinity of the ray Ω. Actually, the DRT system itself represents also the approximate ray tracing system for paraxial rays. For this reason, the dynamic ray tracing is also often called paraxial ray tracing. Here, however, we use the procedure to compute the quantities $\hat{\mathbf{Q}}$, $\hat{\mathbf{P}}$ and $\hat{\mathbf{M}}$ along the ray, not to compute paraxial rays. Therefore, we continue to call it dynamic ray tracing.

As indicated above, instead of the global Cartesian coordinate system, the dynamic ray tracing equations can be expressed in various coordinate systems related to the ray Ω. Among them, the curvilinear **ray-centred coordinate system** q_1, q_2, q_3 is the most common. The basic property of the ray-centred coordinate system is that the ray Ω represents its coordinate axis q_3. The q_1 and q_2 coordinate axes are straight lines situated in the plane tangent to the wavefront at its intersection with the ray Ω, and are mutually perpendicular. Similarly as in ray tracing, we again consider $q_3 = \gamma_3 = \tau$, i.e., q_3 is the travel time along the ray Ω. As the system is curvilinear, we have to distinguish two systems of basis vectors: the contravariant basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ (tangential to coordinate axes), and the covariant basis vectors $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ (perpendicular to coordinate surfaces). At any point on the central ray Ω, the unit contravariant basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ are confined to the plane tangent to the wavefront, and the basis vector $\mathbf{e}_3$ equals $\boldsymbol{\mathcal{U}}$, the ray-velocity vector tangent to the ray. The vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are the basis vectors of the ray-centred coordinate system q_1, q_2, q_3. The covariant basis vectors $\mathbf{f}_1, \mathbf{f}_2$ are perpendicular to the ray Ω, and $\mathbf{f}_3$ equals $\mathbf{p}$, the slowness vector. The contravariant basis vectors $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 = \boldsymbol{\mathcal{U}})$ and the covariant basis vectors $(\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3 = \mathbf{p})$ satisfy mutually the relation

$$\mathbf{e}_i^T \mathbf{f}_j = \delta_{ij} \ . \tag{13}$$

Consequently, $\mathbf{p}^T \mathbf{e}_I = 0$, $\boldsymbol{\mathcal{U}}^T \mathbf{f}_J = 0$ and $\boldsymbol{\mathcal{U}}^T \mathbf{p} = 1$ holds along the whole ray Ω. In inhomogeneous anisotropic media, it is useful to determine first $\mathbf{e}_1$ and $\mathbf{e}_2$ along the ray numerically, and then to determine other quantities from known $\mathbf{e}_1$ and $\mathbf{e}_2$. The relevant differential equation of the first order for $\mathbf{e}_1$ and $\mathbf{e}_2$ is obtained by differentiating relation $\mathbf{p}^T \mathbf{e}_I = 0$:

$$\mathrm{d}\mathbf{e}_I / \mathrm{d}\tau = \mathcal{C}^2 (\mathbf{e}_I^T \boldsymbol{\eta}) \mathbf{p} \ . \tag{14}$$

It is sufficient to compute only one of the unit basis vectors $\mathbf{e}_1, \mathbf{e}_2$, as the other may be determined from the orthogonality relation $\mathbf{e}_2 = \mathcal{C}\mathbf{p} \times \mathbf{e}_1$. The vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathcal{C}\mathbf{p}$, have the following property: once they are unit, mutually perpendicular and right-handed at one point of the ray (say at the initial point $\tau = \tau_0$), they are unit, mutually perpendicular and right handed along the whole ray.

Once $\mathbf{e}_1$ and $\mathbf{e}_2$ are known, we can also simply determine $\mathbf{f}_1, \mathbf{f}_2$ using the relations

$$\mathbf{f}_1 = \frac{\mathbf{e}_2 \times \boldsymbol{\mathcal{U}}}{\boldsymbol{\mathcal{U}}^T (\mathbf{e}_1 \times \mathbf{e}_2)} \ , \quad \mathbf{f}_2 = \frac{\boldsymbol{\mathcal{U}} \times \mathbf{e}_1}{\boldsymbol{\mathcal{U}}^T (\mathbf{e}_1 \times \mathbf{e}_2)} \ . \tag{15}$$

The basis vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ are perpendicular to the ray Ω, see the cross-products of $\mathbf{e}_1, \mathbf{e}_2$ with the ray-velocity vector $\boldsymbol{\mathcal{U}}$ in (15). The basis vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ are not necessarily unit and mutually perpendicular, but $\mathbf{e}_1$ and $\mathbf{e}_2$ are.

In principle, it would be also possible to calculate the basis vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ instead of vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ along the ray. The relevant differential equations would be obtained by differentiating the relation $\boldsymbol{\mathcal{U}}^T \mathbf{f}_J = 0$. The resulting differential equations are, however, more complicated than (14).

Note that the ray-centred coordinate system q_1, q_2, q_3, as introduced here, differs somewhat from the ray-centred coordinate system, which has been routinely used in isotropic inhomogeneous media. First, the coordinate axes q_1 and q_2 are not perpendicular to the ray Ω. Second, the coordinate q_3 is usually taken as the arclenght along the ray in isotropic media. The choice of $q_3 = \tau$, used here, simplifies considerably all computations, as $\partial T/\partial q_n = \delta_{n3}$ and $\partial^2 T/\partial q_3 \partial q_n = 0$ at any point of the ray. The choice of $q_3 = \tau$ was first introduced to ray-centred coordinate system by Klimeš (1994).

The DRT system in ray-centred coordinates can be decoupled into two subsystems. The first subsystem is related only to the coordinates q_1 and q_2 in the plane tangent to the wavefront at its intersection with the ray Ω, not to the coordinate q_3. It provides 2×2 matrices $\mathbf{Q}$ and $\mathbf{P}$, with components

$$Q_{IJ} = \partial q_I/\partial \gamma_J \; , \qquad P_{IJ} = \partial p_I^{(q)}/\partial \gamma_J \; . \tag{16}$$

The DRT system consists of four equations for Q_{IJ} and P_{IJ} specified for one of the two ray parameters γ_J. The symbol $p_I^{(q)}$ denotes the I-th component of the slowness vector $\mathbf{p}$ in the ray-centred coordinate system. Consequently, the whole 2×2 matrices $\mathbf{Q}$ and $\mathbf{P}$ are obtained by solving the DRT system twice, each time with proper initial conditions corresponding to considered γ_J. We can also obtain the 2×2 matrix $\mathbf{M}$ of second derivatives of the travel time T with respect to ray-centred coordinates q_I:

$$M_{IJ} = \frac{\partial^2 T}{\partial q_I \, \partial q_J} \; . \tag{17}$$

Similarly as in equation (12), the 2×2 matrices $\mathbf{Q}$, $\mathbf{P}$ and $\mathbf{M}$ are connected by the relation

$$\mathbf{M} = \mathbf{P}\mathbf{Q}^{-1} \; . \tag{18}$$

The second subsystem is related to the coordinate q_3 and can be solved analytically. We shall not discuss it here.

Several other coordinate systems can be also used in dynamic ray tracing. Instead of ray-centred coordinates q_1, q_2, q_3, we can alternatively use **the wavefront orthonormal coordinates** y_1, y_2, y_3. The wavefront orthonormal coordinates y_1, y_2 coincide with ray-centred coordinates q_1, q_2. The coordinate y_3, however, differs from q_3. The wavefront orthonormal coordinate system is rectangular, and its y_3-axis is a straight line parallel to the slowness vector at a given point of the ray Ω. The dynamic ray tracing for $Q_{IJ}^{(y)}$ and $P_{IJ}^{(y)}$ is the same as for Q_{IJ} and P_{IJ} in ray-centred coordinates given by (16) (although it is expressed in a different way, see Appendix B).

The dynamic ray tracing system in Cartesian coordinates may be simplified to **simplified DRT system in Cartesian coordinates**. In the simplified DRT system, it is necessary to choose special initial conditions, see Section 2.5. Then it is possible to compute only two columns of 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$, not the third columns. Thus, it is not necessary to solve the DRT system three times, but only twice. From these two first columns, however, we can simply determine Q_{IJ} and P_{IJ}, corresponding to DRT in ray-centred coordinates. Consequently, we can proceed exactly in the same way as in ray-centred coordinates, which we describe in the following.

2.3 Ray-theory amplitudes

Let us again consider a harmonic high-frequency seismic body wave propagating in a laterally varying, anisotropic layered structure and the ray Ω corresponding to this wave. The ray-theory displacement vector $\mathbf{u}(\tau)$ at any point τ on the ray Ω is given by the well-known expression:

$$\mathbf{u}(\tau) = A(\tau)\mathbf{g}(\tau)\exp[-\mathrm{i}\omega(t - T(\tau))] \; . \tag{19}$$

Here $A(\tau)$ is a scalar ray-theory amplitude, which is generally complex-valued, $\mathbf{g}(\tau)$ is the real-valued unit polarization vector and $T(\tau) = \tau$ is the travel time on the ray Ω. The travel time and the polarization vector are determined during the ray tracing. It remains to discuss the computation of the scalar ray-theory amplitude $A(\tau)$. For it, we need the DRT. For simplicity, we consider the DRT expressed in the ray-centred coordinates.

The scalar ray-theory amplitude can be determined from the continuation relation along the ray Ω. We consider two points on the ray specified by τ and τ_0, and assume that $A(\tau_0)$ is known. Then the continuation formula reads:

$$A(\tau) = \left[\frac{\rho(\tau_0)\mathcal{C}(\tau_0)}{\rho(\tau)\mathcal{C}(\tau)}\right]^{1/2} \left[\frac{\det \mathbf{Q}(\tau_0)}{\det \mathbf{Q}(\tau)}\right]^{1/2} \mathcal{R}^C A(\tau_0) \; . \tag{20}$$

Continuation relation is regular as long as $\det \mathbf{Q}(\tau)$ is nonzero. In equation (20), ρ is the density, $\mathcal{C}$ the phase velocity (known from ray tracing), $\mathcal{R}^C$ is the complete energy reflection/transmission coefficient along the ray Ω from τ_0 to τ, and $\mathbf{Q}$ is the 2×2 matrix whose elements are defined in eq.(16). The matrix $\mathbf{Q}$ is often called the matrix of geometrical spreading, and the expression $\det \mathbf{Q}$ the geometrical spreading.

The complete energy R/T coefficient $\mathcal{R}^C$ along Ω from τ_0 to τ is a product of plane-wave energy R/T coefficients determined at all points of incidence of the ray Ω on structural interfaces between τ_0 and τ. Mode conversions at individual interfaces are automatically included in $\mathcal{R}^C$. The algorithms for computation of plane-wave energy R/T coefficients at structural interfaces are well known, see e.g. Červený (2001), where other references can be also found. For this reason, we do not discuss these algorithms here. We only note that at the point of incidence, the incident wave and the structural interface are considered to be locally planar, and the media on both sides of the interface are considered to be locally homogeneous. We emphasize that $\mathcal{R}^C$ is a product of the energy R/T coefficients, not of the displacement R/T coefficients. With displacement R/T coefficients, eq.(20) would have a more complicated form.

As we can see from eq.(20), for the determination of ray-theory amplitudes, it is sufficient to know the 2×2 matrix $\mathbf{Q}$. Knowledge of the matrix $\mathbf{P}$, which is determined together with $\mathbf{Q}$ by DRT, is not necessary. It would be, thus, possible to use an alternative version of the DRT system, in which only $\mathbf{Q}$ is computed. Such a dynamic ray tracing system would consist only of one half of ordinary differential equations (for $\mathbf{Q}$), but the equations would be of second order, which are more difficult to solve than the equations of the first order. We prefer the DRT system consisting of differential equations of the first order, which allows construction of the propagator matrix with its broad applications. Moreover, we need the 2×2 matrix $\mathbf{P}$ for the determination of the important matrix $\mathbf{M}$ necessary for the paraxial and Gaussian beam computations.

For the evaluation of the expression (20) for the ray-theory amplitudes, it is not important whether the non-orthogonal ray-centred or the wavefront orthonormal coordinate system is used for DRT. The 2×2 matrix $\mathbf{Q}$ is the same in both systems. In the global Cartesian coordinate system x_i, in which the 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ are used, see (9), the determination of the geometrical spreading would require some modifications. When we use the simplified DRT in Cartesian coordinates, the 2×2 matrices $\mathbf{Q}$ and $\mathbf{P}$ are directly obtained.

It is useful to express (19) with (20) in the following form:

$$\mathbf{u}(\tau) = \mathbf{U}^{\Omega}(\tau) \left[\frac{\det \mathbf{Q}(\tau_0)}{\det \mathbf{Q}(\tau)} \right]^{1/2} \exp[-\mathrm{i}\omega(t - T(\tau))] \ , \tag{21}$$

where $\mathbf{U}^{\Omega}$ is called the vectorial spreading-free amplitude. It is given by the relation

$$\mathbf{U}^{\Omega}(\tau) = \left[\frac{\rho(\tau_0)\mathcal{C}(\tau_0)}{\rho(\tau)\mathcal{C}(\tau)} \right]^{1/2} \mathcal{R}^C A(\tau_0)\mathbf{g}(\tau) \ . \tag{22}$$

The vectorial spreading-free amplitude depends on quantities determined only at points on the ray Ω. It does not depend on the paraxial ray field.

2.4 Ray propagator matrix

In the ray method and its various modifications and extensions, particularly in the paraxial ray method and in the computation of Gaussian beams, a very important role is played by the ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$. Under the ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ we understand the propagator matrix of the system of linear ordinary differential equations of the first order representing the DRT system along the ray Ω. Two basic properties of the DRT system which allow us to construct and exploit the powerful propagator matrix concept are the linearity of the system and the fact that it consists of ordinary differential equations of the first-order. The ray propagator matrix can be computed for the DRT system in global Cartesian coordinates as well as in ray-centred coordinates (and also in wavefront orthonormal coordinates). In global Cartesian coordinates, the ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ is 6×6, in ray-centred coordinates, it reduces to 4×4. Both types of matrices can be used in the ray method computations and in the computations of Gaussian beams. For simplicity, we consider only the 4×4 ray propagator matrices in ray-centred coordinates (or wavefront orthonormal coordinates) in the following. All equations of this section, however, can be also extended for 6×6 propagator matrices.

We introduce the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ as the fundamental matrix of the DRT system

$$\frac{\mathrm{d}\mathbf{\Pi}(\tau, \tau_0)}{\mathrm{d}\tau} = \mathbf{S}(\tau)\mathbf{\Pi}(\tau, \tau_0) \ , \tag{23}$$

which satisfies at $\tau = \tau_0$ the initial condition:

$$\mathbf{\Pi}(\tau_0, \tau_0) = \mathbf{I} \ . \tag{24}$$

Here $\mathbf{S}(\tau)$ is the 4×4 system matrix of the DRT system and $\mathbf{I}$ is the 4×4 identity matrix. Note that the fundamental matrix is a matrix composed of four linearly independent solutions of the DRT system. The linearly independent solutions are guaranteed by the initial conditions (24). The specific expressions, which form the system matrix $\mathbf{S}(\tau)$ of the DRT systems are shown in Appendix B.

Let us emphasize two important facts. First, the four linearly independent solutions of (23) are sought, in fact, for the price of only one solution. The most expensive part in the determination of the system matrix $\mathbf{S}(\tau)$ is evaluation of coefficients of the DRT equations. Once the coefficients are known, it is not a great difference if we seek only one or more solutions of (23). Second, evaluation of coefficients of the DRT system is much faster than evaluation of coefficients of the ray-tracing equations. Except the second-order derivatives of the generalized Christoffel matrix, only the terms already used to determine the right-hand sides of the ray-tracing equations are used.

It is common to express the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ in the following form:

$$\mathbf{\Pi}(\tau,\tau_0) = \begin{pmatrix} \mathbf{Q}_1(\tau,\tau_0) & \mathbf{Q}_2(\tau,\tau_0) \\ \mathbf{P}_1(\tau,\tau_0) & \mathbf{P}_2(\tau,\tau_0) \end{pmatrix} . \tag{25}$$

Here $\mathbf{Q}_1(\tau,\tau_0)$, $\mathbf{Q}_2(\tau,\tau_0)$, $\mathbf{P}_1(\tau,\tau_0)$ and $\mathbf{P}_2(\tau,\tau_0)$ are 2×2 matrices. These matrices have a very simple physical meaning for an orthonomic system of rays, following from (24):

a) $\mathbf{Q}_1(\tau,\tau_0)$ and $\mathbf{P}_1(\tau,\tau_0)$ are solutions of the DRT system for the initial conditions at $\tau=\tau_0$:

$$\mathbf{Q}_1(\tau_0,\tau_0) = \mathbf{I} \ , \quad \mathbf{P}_1(\tau_0,\tau_0) = \mathbf{0} \ . \tag{26}$$

In (26), $\mathbf{I}$ is the 2×2 identity matrix and $\mathbf{0}$ is the 2×2 null matrix. It is easy to see that these initial conditions correspond to a plane wavefront at $\tau=\tau_0$.

b) $\mathbf{Q}_2(\tau,\tau_0)$ and $\mathbf{P}_2(\tau,\tau_0)$ are solutions of the DRT system for the initial conditions at $\tau=\tau_0$:

$$\mathbf{Q}_2(\tau_0,\tau_0) = \mathbf{0} \ , \quad \mathbf{P}_2(\tau_0,\tau_0) = \mathbf{I} \ . \tag{27}$$

It is easy to see that in this case the initial conditions correspond to a point source at $\tau=\tau_0$.

Thus, the ray propagator matrix is determined if the DRT system is solved four times: twice with the plane-wave initial conditions corresponding to (26) and twice with the point-source initial conditions corresponding to (27). Alternatively, we can say that the DRT system should be solved four times, with initial conditions specified by four columns of the 4×4 identity matrix.

Once we know the ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$, we can determine the solution of DRT system for arbitrary initial conditions specified by 2×2 matrices $\mathbf{Q}(\tau_0)$ and $\mathbf{P}(\tau_0)$ by a single matrix operation:

$$\begin{pmatrix} \mathbf{Q}(\tau) \\ \mathbf{P}(\tau) \end{pmatrix} = \mathbf{\Pi}(\tau,\tau_0) \begin{pmatrix} \mathbf{Q}(\tau_0) \\ \mathbf{P}(\tau_0) \end{pmatrix} . \tag{28}$$

The 4×4 ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ has many important and interesting properties, which can be conveniently used in the theory of Gaussian beams. These properties are briefly described in Appendix C.

Let us mention that we can seek the solution of the DRT system without constructing the ray propagator matrix, by only specifying the specific initial conditions of the DRT system. This may reduce computational efforts, but reduces considerably the flexibility, which use of the ray propagator matrix offers. See more details in Appendix D.

The ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ can be used to construct a simple analytical relation for the continuation of the 2×2 matrix $\mathbf{M}$ of second spatial derivatives of the travel-time field along the ray Ω. Using (18) and (28), we obtain

$$\mathbf{M}(\tau) = \mathbf{P}(\tau)\mathbf{Q}^{-1}(\tau) = [\mathbf{P}_1(\tau, \tau_0) + \mathbf{P}_2(\tau, \tau_0)\mathbf{M}(\tau_0)][\mathbf{Q}_1(\tau, \tau_0) + \mathbf{Q}_2(\tau, \tau_0)\mathbf{M}(\tau_0)]^{-1} \; . \quad (29)$$

This is a very important relation in the theory of Gaussian beams. Once we know the ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ along the ray Ω, and the matrix $\mathbf{M}(\tau_0)$ at the point of the ray Ω with $\tau = \tau_0$, equation (29) provides a simple way to determine $\mathbf{M}(\tau)$ for arbitrary τ along the ray Ω. If we use the interface propagator matrix in $\mathbf{\Pi}(\tau, \tau_0)$, see (C-7), equation (29) can also be used along a ray of a wave reflected or transmitted at a structural interface.

Another important application of the ray-propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ is in the transformation of the factor $[\det \mathbf{Q}(\tau_0)/\det \mathbf{Q}(\tau)]^{1/2}$ appearing in the formula for ray-theory amplitudes, see eq.(21). We obtain

$$[\det \mathbf{Q}(\tau_0)/\det \mathbf{Q}(\tau)]^{1/2} = [\det \Big(\mathbf{Q}_1(\tau, \tau_0) + \mathbf{Q}_2(\tau, \tau_0)\mathbf{M}(\tau_0)\Big)]^{-1/2} \; . \quad (30)$$

Similarly as equation (29), eq.(30) plays an important role in the theory of Gaussian beams. Great advantage of the expression on the right-hand side of eq.(30) is that it is expressed in terms of known elements ($\mathbf{Q}_1$, $\mathbf{Q}_2$) of the propagator matrix and of physically well understandable initial conditions, namely in terms of the matrix of second spatial derivatives of the travel time field $\mathbf{M}(\tau_0)$. No other initial values are required.

2.5 Simplified DRT in Cartesian coordinates

Solving the DRT system in Cartesian coordinates six times, with initial conditions specified by columns of the 6×6 identity matrix, we can determine the 6×6 ray propagator matrix in Cartesian coordinates, from which the solution of the DRT system for any initial conditions can be obtained.

We can, however, simplify the solution of DRT in Cartesian coordinates. In fact, when we choose suitably the initial conditions for DRT, it is sufficient to compute only the first two columns of the 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ along a given ray Ω. This simplified version of DRT does not allow us to determine the 6×6 ray propagator matrix in Cartesian coordinates x_i, but it can be used to determine the 4×4 ray propagator matrix in wavefront orthonormal coordinates y_I, at any point of the ray Ω. The 4×4 ray propagator matrix also automatically represents the 4×4 ray propagator matrix in ray-centred coordinates. The solution of the simplified DRT system in Cartesian coordinates is quite sufficient for the determination of paraxial travel times and Gaussian beams. The advantage of this approach is that we need to solve the DRT system only four times, not six times.

Let us denote here the 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$ obtained by DRT in Cartesian coordinates with the superscript notation (x), and the 2×2 matrices $\mathbf{Q}$ and $\mathbf{P}$ obtained by DRT in wavefront orthonormal coordinates with the superscript notation (y). Consequently, the elements in first two columns of $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ are $Q^{(x)}_{iN}$ and $P^{(x)}_{iN}$, $i = 1, 2, 3$, $N = 1, 2$. Similarly, the elements of the 2×2 matrices $\mathbf{Q}^{(y)}$ and $\mathbf{P}^{(y)}$ are $Q^{(y)}_{JK}$ and $P^{(y)}_{JK}$; $J, K = 1, 2$. The transformation relations between the elements $Q^{(x)}_{iN}$, $P^{(x)}_{iN}$ and $Q^{(y)}_{IJ}$, $P^{(y)}_{IJ}$ are derived in Červený (2001, p. 270):

$$\begin{aligned} Q^{(x)}_{iN} &= e_{Ji} Q^{(y)}_{JN} \ , \\ P^{(x)}_{iN} &= e_{Ij} p_i \eta_j Q^{(y)}_{IN} + (e_{Ii} - e_{Ij} p_i \mathcal{U}_j) P^{(y)}_{IN} \ . \end{aligned} \tag{31}$$

The reverse transformation reads

$$Q^{(y)}_{JK} = e_{Jl} Q^{(x)}_{lK} \ , \qquad P^{(y)}_{JK} = e_{Jl} P^{(x)}_{lK} \ . \tag{32}$$

Here the components of vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{p}$, $\boldsymbol{\eta}$ and $\boldsymbol{\mathcal{U}}$ are expressed in Cartesian coordinates.

The important problem is how to specify the initial conditions for DRT in Cartesian coordinates, when we wish to compute the 4×4 ray propagator matrix $\mathbf{\Pi}^{(y)}(\tau, \tau_0)$ corresponding to wavefront orthonormal coordinates. For a point-source initial conditions at $\tau = \tau_0$, we put $Q^{(y)}_{IK}(\tau_0) = 0$ and $P^{(y)}_{JK}(\tau_0) = \delta_{JK}$, see (27). Then the initial conditions for $Q^{(x)}_{iN}(\tau)$ and $P^{(x)}_{iN}(\tau_0)$ follow from (31):

$$Q^{(x)}_{iN}(\tau_0) = 0 \ , \qquad P^{(x)}_{iN}(\tau_0) = e_{Ni} - e_{Nj} p_i \mathcal{U}_j \ . \tag{33}$$

Similarly, for plane-wave initial conditions at $\tau = \tau_0$, we put $Q^{(y)}_{IN}(\tau_0) = \delta_{IN}$, $P^{(y)}_{IN}(\tau_0) = 0$, see (26). Inserting these initial conditions to (31) yields

$$Q^{(x)}_{iN}(\tau_0) = e_{Ni} \ , \qquad P^{(y)}_{iN} = e_{Nj} p_i \eta_j \ . \tag{34}$$

Solving the simplified DRT in Cartesian coordinates twice, with point-source initial conditions (33), for $N = 1$ and $N = 2$, we obtain 12 quantities $Q^{(x)}_{iN}(\tau)$ and $P^{(x)}_{iN}(\tau)$ at any point τ of the ray Ω. Similarly, if we consider the plane wave initial conditions (34), again for $N = 1$ and $N = 2$, we obtain other 12 quantities. All these quantities may be transformed from Cartesian to wavefront orthonormal coordinates using (32). In this way, we obtain the 4×4 ray-propagator matrix $\mathbf{\Pi}^{(y)}(\tau, \tau_0)$, necessary for computation of paraxial travel times and Gaussian beams.

Let us note that the simplified DRT system in Cartesian coordinates can be very efficiently used for the Gaussian beam computations with such codes like ANRAY (Gajewski and Pšenčík, 1991). In fact, the simplified Cartesian DRT system with point-source initial conditions (33) has been already used in ANRAY, see Pšenčík and Teles (1996). In order to generalize ANRAY for Gaussian beam computations, it will be sufficient to solve the simplified DRT system also for the initial conditions (34).

3 Paraxial ray approximation

The solution of the DRT system and the computations of the ray-propagator matrix considerably extend the possibilities of the ray method. The most important extension consists in the possibility to compute approximately the travel time field T in the "paraxial" vicinity of the ray Ω, not only along the ray Ω itself. We call such travel times the paraxial travel times. The knowledge of the real-valued paraxial travel times is a necessary prerequisite of many other extensions of the ray method. For this reason, we shall first derive useful expressions for the real-valued paraxial travel times. After this, we shall use the expressions for paraxial travel times in the equations for the relevant displacement vector and obtain the so-called paraxial approximation of the displacement vector. The paraxial approximation of the displacement vector represents the corner stone in the computation of Chapman-Maslov synthetic seismograms (Chapman and Drummond, 1982; Thomson and Chapman, 1985; Chapman, 2004). The next extension is from the real-valued to complex-valued paraxial travel times, which leads to Gaussian beams. This extension is very simple: We merely allow the initial 2×2 matrix $\mathbf{M}(\tau)$ of the second derivatives of the travel time field with respect to the ray-centred coordinates to be complex-valued, and specify certain conditions that complex-valued $\mathbf{M}(\tau_0)$ must satisfy. The ray Ω, the ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ and the travel time along the ray Ω remain real-valued, see Section 4.

3.1 Paraxial travel times

Paraxial travel times are usually specified by quadratic expansions of travel time T at points situated on the ray Ω.

Let us first consider the global Cartesian coordinate system x_i and choose any point R_Ω situated on the ray Ω. We further specify any point R situated in the vicinity of R_Ω. The point R is in general situated outside the ray Ω, but may be also situated on it. Then the paraxial travel time $T(R, R_\Omega)$ in the vicinity of R_Ω can be expressed in terms of $T(R_\Omega)$ using the following local quadratic expansion at R_Ω:

$$\begin{aligned} T(R, R_\Omega) &= T(R_\Omega) + (\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T \mathbf{p}(R_\Omega) \\ &+ \tfrac{1}{2}(\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T \hat{\mathbf{M}}(R_\Omega)(\mathbf{x}(R) - \mathbf{x}(R_\Omega)) \ . \end{aligned} \tag{35}$$

The travel time $T(R_\Omega)$ and the slowness vector $\mathbf{p}(R_\Omega)$ are known from ray tracing of the ray Ω. The 3×3 matrix $\hat{\mathbf{M}}(R_\Omega)$ of the second derivatives of the travel-time field in global Cartesian coordinates can be calculated using the 6×6 ray-propagator matrix, computed by DRT.

A similar expansion for the paraxial travel time $T(R, R_\Omega)$ may be written also in other coordinate systems, e.g. in ray-centred coordinates q_1, q_2, q_3, or in the wavefront orthonormal coordinate system y_1, y_2, y_3, connected with the ray Ω. We shall first consider the ray-centred coordinate system q_i. The ray Ω is the q_3-axis of the ray-centred coordinate system, with $q_3 = \tau$. The other two coordinates q_1, q_2 of the ray-centred coordinate system are zero along Ω, so that the ray-centred coordinates of R_Ω are $(0, 0, q_3 = \tau)$. The ray-centred coordinates $\mathbf{q} \equiv (q_1, q_2)^T$ are Cartesian coordinates in the plane tangent to the wavefront at R_Ω, with the origin at R_Ω. Then the paraxial travel time $T(R, R_\Omega)$ at the point $R(q_1, q_2, q_3 = \tau)$ can be expressed in terms of $T(R_\Omega)$ as follows:

$$T(R, R_\Omega) = T(R_\Omega) + \tfrac{1}{2}\mathbf{q}^T(R)\mathbf{M}(R_\Omega)\mathbf{q}(R) \ . \tag{36}$$

The linear term $\mathbf{q}(R)\mathbf{p}^{(q)}(R_\Omega)$ in (36) is absent, as the ray-centred components of the slowness vector, $p_1^{(q)}(R_\Omega)$ and $p_2^{(q)}(R_\Omega)$ at R_Ω on Ω are zero (the slowness vector is perpendicular to the wavefront). For a given initial 2×2 matrix $\mathbf{M}(\tau_0)$, the 2×2 matrix $\mathbf{M}(R_\Omega)$ of the second derivatives of the travel-time field at the point R_Ω on the ray Ω in ray-centred coordinates q_1, q_2 is computed from the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ in ray-centred coordinates using (29).

Equation (36) for the paraxial travel time in ray-centred coordinates is very simple, indeed. It uses only the 2×2 matrix $\mathbf{M}(R_\Omega) \equiv \mathbf{M}(\tau)$. Moreover, it does not contain any linear term.

We now assume that the basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ are determined along the ray Ω using equations (14). Then equation (36) for the paraxial travel times in ray-centred coordinates q_1, q_2 is exactly the same as analogous equations for paraxial travel times in wavefront orthonormal coordinates y_1, y_2:

$$T(R, R_\Omega) = T(R_\Omega) + \tfrac{1}{2}\mathbf{y}^T(R)\mathbf{M}(R_\Omega)\mathbf{y}(R) \ . \tag{37}$$

Here $\mathbf{y} = (y_1, y_2)^T$. The equivalence of (36) and (37) is not surprising. The dynamic ray tracing system, the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ and the 2×2 matrix $\mathbf{M}(R_\Omega)$ in ray-centred coordinates q_1, q_2 are exactly the same as in wavefront orthonormal coordinates y_1, y_2. Only when we use equations involving the third coordinates (q_3 or y_3), the equations become different. The basis vector $\mathbf{e}_3$ in the ray-centred coordinates is a vector tangent to the ray, but the basis vector $\mathbf{e}_3^{(y)}$ in orthonormal wavefront coordinates is parallel to the slowness vector $\mathbf{p}(R_\Omega)$. Moreover, the dimension of q_3 is time, whereas the dimension of y_3 is length.

In the following sections, we shall consider coordinates q_1, q_2 of the ray-centred coordinate system. All presented equations are, however, valid even in coordinates y_1, y_2 of the wavefront orthonormal coordinate system.

3.2 Paraxial approximation of the displacement vector

In this section, we discuss extension of the ray-theory expression for the displacement vector (21), by including the paraxial travel times (36). Consequently, the resulting expression gives travel times not only along the ray Ω, but also in its paraxial vicinity. In ray-centred coordinates $q_1, q_2, q_3 = \tau$, we obtain

$$\begin{aligned} \mathbf{u}^{par}(q_1, q_2, \tau) &= \mathbf{U}^\Omega(\tau)[\det(\mathbf{Q}_1(\tau, \tau_0) + \mathbf{Q}_2(\tau, \tau_0)\mathbf{M}(\tau_0))]^{-1/2} \\ &\times \ \exp[-\mathrm{i}\omega(t - T(\tau) - \tfrac{1}{2}\mathbf{q}^T\mathbf{M}(\tau)\mathbf{q})] \ . \end{aligned} \tag{38}$$

Here $\mathbf{q} \equiv (q_1, q_2)^T$ are ray-centred coordinates, $\mathbf{U}^\Omega(\tau)$ is the spreading-free amplitude, given by (22), and $\mathbf{M}(\tau)$ is the 2×2 matrix of second derivatives of the travel-time field in ray-centred coordinates given by equation (29). The factor $[\det(\mathbf{Q}_1(\tau, \tau_0) + \mathbf{Q}_2(\tau, \tau_0)\mathbf{M}(\tau_0))]^{-1/2}$ is actually equivalent to $[\det(\mathbf{Q}(\tau_0)/\det\mathbf{Q}(\tau))]^{1/2}$ used in (21), but it uses the 2×2 matrices $\mathbf{Q}_1(\tau, \tau_0)$ and $\mathbf{Q}_2(\tau, \tau_0)$, see eq. (25), needed in the computation of $\mathbf{M}(\tau)$. Consequently, it does not require any additional computations.

As we can see, the computation of paraxial approximation of the displacement vector (38) requires the specification of an additional initial condition to the standard ray-theory expressions, namely the specification of the 2×2 matrix $\mathbf{M}(\tau_0)$ of second derivatives of the travel-time field at an arbitrary point of the ray Ω, $\tau = \tau_0$. No separate initial conditions for $\mathbf{Q}(\tau_0)$ and $\mathbf{P}(\tau_0)$ are required. Fortunately, the 2×2 matrix $\mathbf{M}(\tau_0)$ is physically simply understandable, and can be expressed in terms of the curvature matrix of the wavefront at τ_0. Note that the 2×2 matrix $\mathbf{M}(\tau_0)$ must be symmetric and finite.

Similar expression for paraxial approximation of the displacement vector as (38) can be also derived in global Cartesian coordinates. We do not present it here, as we will not use it. If we use the wavefront orthonormal coordinates y_1, y_2, the final expression would remain exactly the same as in (38).

In equation (38), we expanded the travel time T from the central ray Ω to the paraxial vicinity of Ω. We, however, did not expand the ray-theory amplitudes in the vicinity of Ω; they are left the same as on the ray Ω. The expansion of the ray-theory amplitudes into the paraxial region for layered, isotropic or anisotropic media would be considerably more complicated, and cannot be derived in the framework of standard DRT. It would require to develop higher-order paraxial methods. Such higher-order paraxial methods, however, have not yet been investigated.

The other possibility how to improve the paraxial ray-theory amplitudes is to trace some auxiliary rays in the vicinity of Ω and to take them into account in the computation of paraxial amplitudes. Actually, the most efficient and accurate way consists in the computation of weighted summation of paraxial approximations of the displacement vector (38), or of paraxial approximations of the displacement vector in global Cartesian coordinates, concentrated close to rays distributed densely in the region of interest. In the global Cartesian coordinates, such method derived in a more sophisticated way, has been usually called the Chapman-Maslov method.

4 Gaussian beams

4.1 Gaussian beams in ray-centred coordinates

We consider a real-valued ray Ω, situated in an inhomogeneous anisotropic layered medium. We assume that the dynamic ray tracing in ray-centred coordinates q_1, q_2 has been performed along the ray Ω and that the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ has been determined. The 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ and its 2×2 submatrices $\mathbf{Q}_1(\tau, \tau_0)$, $\mathbf{Q}_2(\tau, \tau_0)$, $\mathbf{P}_1(\tau, \tau_0)$ and $\mathbf{P}_2(\tau, \tau_0)$ are real-valued. If we use equation (38) for paraxial approximation of the displacement vector, we can use freely the initial 2×2 real-valued matrix $\mathbf{M}(\tau_0)$ of second derivatives of the travel-time field. We only require that $\mathbf{M}(\tau_0)$ is real-valued, symmetric and finite.

In equation (38), however, we can also consider $\mathbf{M}(\tau_0)$ complex-valued,

$$\mathbf{M}(\tau_0) = \mathrm{Re}\mathbf{M}(\tau_0) + \mathrm{i}\mathrm{Im}\mathbf{M}(\tau_0) \ . \qquad (39)$$

If we require that such 2×2 matrix $\mathbf{M}(\tau_0)$ satisfies the following conditions: a) the 2×2 matrix $\mathbf{M}(\tau_0)$ is symmetric, b) the 2×2 matrix $\mathbf{M}(\tau_0)$ is finite, c) the 2×2 matrix

$\mathrm{Im}\mathbf{M}(\tau_0)$ is positive definite, then we obtain from (38) a solution, which has been usually called the Gaussian beam:

$$\begin{aligned} \mathbf{u}^{beam}(q_1,q_2,\tau) &= \mathbf{U}^{\Omega}(\tau)(\det\mathbf{W})^{-1/2}\exp[-\tfrac{1}{2}\omega\mathbf{q}^T\mathrm{Im}\mathbf{M}(\tau)\mathbf{q}] \\ &\times\ \exp[-\mathrm{i}\omega(t-T(\tau)-\tfrac{1}{2}\mathbf{q}^T\mathrm{Re}\mathbf{M}(\tau)\mathbf{q})]\ . \end{aligned} \tag{40}$$

Here $\mathbf{q}=(q_1,q_2)^T$ and

$$\mathbf{W}(\tau,\tau_0)=\mathbf{Q}_1(\tau,\tau_0)+\mathbf{Q}_2(\tau,\tau_0)(\mathrm{Re}\mathbf{M}(\tau_0)+\mathrm{i}\mathrm{Im}\mathbf{M}(\tau_0))\ . \tag{41}$$

The conditions a)-c) given above are known as Gaussian beam existence conditions. The properties of the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ along the ray Ω then guarantee that the 2×2 complex-valued matrix $\mathbf{M}(\tau)$ satisfies the same properties a)-c) along the whole ray Ω. Consequently, the 2×2 matrix $\mathbf{M}(\tau)$ is symmetric and finite at any point τ of the ray Ω, and $\mathrm{Im}\mathbf{M}(\tau)$ is positive definite, again at any point of the ray Ω. Once a Gaussian beam, always a Gaussian beam!

The Gaussian beam existence conditions guarantee that $\mathbf{M}(\tau)$ is finite along the whole ray Ω. This further guarantees that $\det\mathbf{Q}(\tau)$ cannot be zero at any point of the ray Ω, including the point $\tau=\tau_0$. Consequently, the matrix $\mathbf{W}(\tau,\tau_0)$ is regular for any τ. For $\tau=\tau_0$, we have $\mathbf{Q}_1(\tau_0,\tau_0)=\mathbf{I}$, $\mathbf{Q}_2(\tau_0,\tau_0)=\mathbf{0}$, so that

$$\mathbf{W}(\tau_0,\tau_0)=\mathbf{I}\ . \tag{42}$$

As $(\det\mathbf{W}(\tau,\tau_0))^{1/2}$ is, in general, a complex-valued root, we must be careful how to choose its argument. We can determine it in the following way: 1) It equals zero for $\tau=\tau_0$; b) It varies continuously along the ray Ω.

There are no points along the ray Ω, at which $\det\mathbf{W}(\tau,\tau_0)$ is zero. Thus, the use of Gaussian beams removes the singularities at *caustic points*. This is a very important and useful property of Gaussian beams. The problem of caustics is one of the most serious problems in the computation of ray synthetic seismic wave fields in inhomogeneous isotropic or anisotropic media. The method based on the summation of Gaussian beams can be used to remove this problem.

As the Gaussian beams cannot be singular at any point of the ray, they cannot be singular at the initial point τ_0 of the ray. Consequently, the wave field generated by a point source cannot be described by an individual Gaussian beam. It can be, however, described by a weighted sum of Gaussian beams.

Consider again a real-valued ray Ω. Each Gaussian beam connected with this ray is specified by a 2×2 symmetric complex-valued matrix $\mathbf{M}(\tau_0)$ given at an arbitrary point of the ray, $\tau=\tau_0$. Consequently, we can construct a six-parametric system of Gaussian beams connected with the ray Ω. The three parameters $\mathrm{Re}M_{11}(\tau_0)$, $\mathrm{Re}M_{22}(\tau_0)$, and $\mathrm{Re}M_{12}(\tau_0)$, control the shape of the phase front of a Gaussian beam at τ_0. The other three parameters, $\mathrm{Im}M_{11}(\tau_0)$, $\mathrm{Im}M_{22}(\tau_0)$ and $\mathrm{Im}M_{12}(\tau_0)$, control the width of the Gaussian beam at τ_0. The real-valued travel time along the ray Ω and the spreading-free amplitudes $\mathbf{U}^{\Omega}$ are the same for all the Gaussian beams connected with the ray Ω.

Similarly as in paraxial approximation of the displacement vector (38), the ray-theory amplitudes in the expression (40) for Gaussian beams are the same in the whole plane tangent to the wavefront at τ on Ω as at τ. The most efficient and accurate way how to take into account the paraxial changes of ray-theory amplitudes consists in the weighted summation of Gaussian beams (40).

In this section, we have explained how the Gaussian beams in ray-centered coordinates can be computed using the 4×4 real-valued ray-propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$. The complex-valued matrix $\mathbf{M}(\tau)$ and the complex-valued expression $[\det \mathbf{Q}(\tau_0)/\det \mathbf{Q}(\tau)]^{1/2}$, needed in the expression for Gaussian beams, are computed from $\mathbf{\Pi}(\tau,\tau_0)$ using relations (29) and (30). We only choose complex-valued $\mathbf{M}(\tau_0)$ to satisfy the Gaussian beam existence conditions at the point $\tau = \tau_0$. Alternatively, we can avoid the computation of the ray-propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$, and compute the complex-valued matrix $\mathbf{M}(\tau)$ and the complex-valued expression $[\det \mathbf{Q}(\tau_0)/\det \mathbf{Q}(\tau)]^{1/2}$ along the ray Ω directly by solving the dynamic ray tracing with complex-valued initial conditions. See more details in Appendix D.

4.2 Gaussian beams in Cartesian coordinates

Equation (40) with (41) can be simply used to calculate Gaussian beam connected with the ray Ω at any point R, situated in a paraxial vicinity of Ω, in the plane tangent to the wavefront at a **known** point R_Ω on Ω. The position of the point R_Ω on Ω is specified by the monotonic parameter τ and by $q_1 = q_2 = 0$. The ray-centred coordinates q_1, q_2 of the point R are then determined in the plane tangent to the wavefront at R_Ω. This plane is specified by the known basis vectors $\mathbf{e}_1(\tau)$, $\mathbf{e}_2(\tau)$. If we wish, we can then determine the Cartesian coordinates of the point R from Cartesian coordinates of R_Ω, and Cartesian components of $\mathbf{e}_1(\tau)$ and $\mathbf{e}_2(\tau)$.

In various applications, however, it is very useful to specify the point R in Cartesian coordinates directly. For example, such a specification of the observation point R in Cartesian coordinates would be very useful in the summation of Gaussian beams at an observation point R. Then we would meet a considerably more complicated problem to determine the position of the point R_Ω on Ω, which is situated in the plane tangent to the wavefront at R_Ω and containing the observation point R.. Once the point R_Ω is determined, the remaining part of the procedure is easy.

Determination of R_Ω from known R in an inhomogeneous anisotropic medium is very cumbersome. It is cumbersome even in an isotropic inhomogeneous medium, when the plane tangent to the wavefront at R_Ω reduces to the plane normal to Ω at R_Ω. Consequently, in inhomogeneous isotropic media, the solution of the problem requires the numerical determination of the plane perpendicular to Ω, which passes through the point R. For an inhomogeneous anisotropic medium, however, the problem is not purely geometrical since the plane perpendicular to Ω must be replaced by the plane tangent to the wavefront at its intersection with the ray Ω.

To avoid this cumbersome procedure, a local Cartesian coordinate system with its origin at R_Ω on Ω, chosen arbitrarily, but as close as possible to R, has been broadly used in the summation of Gaussian beams in inhomogeneous isotropic media. The same approach can be used in inhomogeneous anisotropic media. It is then simple to transform the local Cartesian coordinates to the global ones. The quadratic expansion of the travel time is used not only with respect to paraxial distances from the ray Ω, but also with respect to distances between R and R_Ω along the ray Ω.

Once we know the sought quantities in the local coordinates with their origin at R_Ω, we can transform them to global Cartesian coordinates x_i, and to determine the paraxial travel times, Gaussian beams and other quantities of our interest in global Cartesian coordinates. For example, when we introduce the local Cartesian coordinate system at the termination of the ray Ω, we can transform it to the global Cartesian coordinate system, and determine the contribution of the Gaussian beam (connected with the ray Ω) at any point $R(x_i)$, situated in the vicinity of the termination point. If the termination points of different rays are situated along some surface, the summation of Gaussian beams can be performed along the target surface. It is no more necessary that the point R is situated in the plane tangent to the wavefront at R_Ω on Ω. This increases considerably the efficiency of the procedure of the summation of Gaussian beams.

Here we present the transformation relation between $\partial^2 T/\partial q_I \partial q_J$, expressed by DRT in ray-centred coordinates, and $\partial^2 T/\partial x_i \partial x_j$, expressed in Cartesian coordinates. This relation is very useful when we perform computations in ray centred coordinates, but wish to transform the results into a local Cartesian coordinate system with its origin at an arbitrary point R_Ω on the ray Ω. A detailed derivation and explanation can be found in Červený and Klimeš (2009). The expression uses only the quantities computed by ray tracing and dynamic ray tracing in ray-centred coordinates q_i at R_Ω. We denote by $\hat{\mathbf{M}}^{(x)}$ the 3×3 matrix with elements $\partial^2 T/\partial x_i \partial x_j$, and by $\mathbf{M}^{(\mathbf{q})}$ the 2×2 matrix with elements $\partial^2 T/\partial q_N \partial q_M$. Then the relation between $\hat{\mathbf{M}}^{(x)}$ and $\mathbf{M}^{(\mathbf{q})}$ at an arbitrary point τ on the ray Ω is as follows:

$$\hat{\mathbf{M}}^{(x)} = \mathbf{f}\ \mathbf{M}^{(q)}\ \mathbf{f}^T + \mathbf{p}\boldsymbol{\eta}^T + \boldsymbol{\eta}\mathbf{p}^T - \mathbf{p}\mathbf{p}^T(\boldsymbol{\mathcal{U}}^T\boldsymbol{\eta}) \ . \tag{43}$$

Here the slowness vector $\mathbf{p}(\tau)$, the ray-velocity vector $\boldsymbol{\mathcal{U}}(\tau)$, and the vector $\boldsymbol{\eta}(\tau)$ are expressed in global Cartesian coordinates. Actually, the Cartesian components of these real-valued vectors are known at any point of the ray Ω, even if the dynamic ray tracing in ray-centred coordinates is used. The vectors $\mathbf{p}(\tau)$, $\boldsymbol{\mathcal{U}}(\tau)$ and $\boldsymbol{\eta}(\tau)$ are known from ray tracing. The symbol $\mathbf{f}$ denotes the 3×2 matrix $\mathbf{f} = (\mathbf{f}_1, \mathbf{f}_2)$. The vectors $\mathbf{f}_1(\tau)$ and $\mathbf{f}_2(\tau)$ can be simply calculated from known vectors $\mathbf{e}_1(\tau)$ and $\mathbf{e}_2(\tau)$ using (15). They are perpendicular to the central ray Ω, in contrast to $\mathbf{e}_1(\tau)$ and $\mathbf{e}_2(\tau)$, which are perpendicular to the slowness vector $\mathbf{p}(\tau)$. The 2×2 matrix $\mathbf{M}^{(q)}$ is the complex-valued matrix of second-order derivatives of the travel time field with respect to ray-centred coordinates, with elements $\partial^2 T/\partial q_I \partial q_J$. The elements are obtained from the dynamic ray tracing in ray-centred coordinates.

Using (43), we obtain the quadratic expansion of the paraxial travel time field in global Cartesian coordinates at an arbitrary point $\mathbf{x}(R)$, situated in the vicinity of the point $\mathbf{x}(R_\Omega)$, chosen arbitrarily on the ray Ω:

$$\begin{aligned} T(R, R_\Omega) &= T(R_\Omega) + (\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T \mathbf{p}(R_\Omega) \\ &+ \tfrac{1}{2}(\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T \hat{\mathbf{M}}^{(x)}(R_\Omega)(\mathbf{x}(R) - \mathbf{x}(R_\Omega)) \ . \end{aligned} \tag{44}$$

The elements of the 3×3 matrix $\hat{\mathbf{M}}^{(x)}(R_\Omega)$ are given by (43). The only complex-valued expression in (44) is the 2×2 matrix $\mathbf{M}^{(q)}(R_\Omega)$, included in the 3×3 matrix $\hat{\mathbf{M}}^{(x)}(R_\Omega)$, see (43).

Now we shall consider a Gaussian beam, connected with the ray Ω, and determine its contribution at the paraxial point R specified in Cartesian coordinates and situated in the vicinity of the point R_Ω on Ω. The point R_Ω corresponds to the sampling parameter $\gamma_3 = \tau$ along Ω. The coordinates of the point R_Ω can be, of course, expressed also in Cartesian coordinates. To some extent, point R_Ω may be chosen arbitrarily on the ray Ω, but must be close to R. Then the contribution of the Gaussian beam, evaluated along Ω, at the point R is as follows:

$$\begin{aligned} \mathbf{u}^{beam}(R) &= \mathbf{U}^{\Omega}(R_\Omega)(\det \mathbf{W})^{-1/2} \exp[-\omega \mathrm{Im} T(R, R_\Omega)] \\ &\times \exp[-\mathrm{i}\omega(t - \mathrm{Re} T(R, R_\Omega))] \ . \end{aligned} \tag{45}$$

Here $\mathbf{U}^{\Omega}$ and $\det \mathbf{W}$ have the same meaning as in equations (40) and (41). The complex-valued paraxial travel time $T(R, R_\Omega)$ is given by (44) with (43). The expression for $\mathrm{Im}T(R, R_\Omega)$ can be simplified, as the only complex-valued quantity in (44) and (43) is the 2×2 matrix $\mathbf{M}^{(q)}(\tau)$, with elements $\partial^2 T/\partial q_N \partial q_M$.

For completeness, we present here the expressions for $\mathrm{Re}T(R, R_\Omega)$ and $\mathrm{Im}T(R, R_\Omega)$:

$$\mathrm{Re}T(R, R_\Omega) = T(R_\Omega) + \tilde{p} + \frac{1}{2}\tilde{\mathbf{f}}\, \mathrm{Re}\mathbf{M}^{(q)}(R_\Omega)\, \tilde{\mathbf{f}}^T + \tilde{p}\tilde{\eta} + \frac{1}{2}(\boldsymbol{\mathcal{U}}^T \boldsymbol{\eta})\tilde{p}^2 \ , \tag{46}$$

$$\mathrm{Im}T(R, R_\Omega) = \frac{1}{2}\tilde{\mathbf{f}}\, \mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)\, \tilde{\mathbf{f}}^T \ . \tag{47}$$

Here

$$\begin{aligned} \tilde{p} &= (\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T \mathbf{p}(R_\Omega) \ , \\ \tilde{\eta} &= (\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T \boldsymbol{\eta}(R_\Omega) \ , \\ \tilde{\mathbf{f}} &= (\tilde{f}_1, \tilde{f}_2) = (\mathbf{x}(R) - \mathbf{x}(R_\Omega))^T (\mathbf{f}_1, \mathbf{f}_2) \ . \end{aligned} \tag{48}$$

The quantities $\tilde{p}$ and $\tilde{\eta}$ represent scalar products of vectors $\mathbf{p}(R_\Omega)$ and $\boldsymbol{\eta}(R_\Omega)$ with the "observation vector" $\mathbf{x}(R) - \mathbf{x}(R_\Omega)$. The 2×1 matrix $\tilde{\mathbf{f}}$ with elements $\tilde{f}_1$ and $\tilde{f}_2$ represents scalar products of vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ with the observation vector $\mathbf{x}(R) - \mathbf{x}(R_\Omega)$. The 2×2 matrix $\mathbf{M}^{(q)}(R_\Omega)$, with elements $M^{(q)}_{IJ}(R_\Omega)$, is known from dynamic ray tracing in ray-centred coordinates. Alternatively, it may be determined by dynamic ray tracing in wavefront orthonormal coordinates, or by simplified dynamic ray tracing in Cartesian coordinates.

In the described approach, we calculate the paraxial travel-time field (44) and the Gaussian beam (45) in Cartesian coordinates, although the dynamic ray tracing has been performed in ray-centred coordinates. We only apply locally (43) at the point R_Ω on the ray Ω, close to the observation point R.

We can, of course, also use an alternative approach, based fully on the dynamic ray tracing in Cartesian coordinates. More specifically, we first compute the 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$, analogous to (25), with the initial conditions specified by columns of the 6×6 identity matrix. The 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tau)$ of second derivatives of the travel time field with respect to Cartesian coordinates is then given by formula analogous to (29), where all the matrices are 3×3, and have a superscript $^{(x)}$.

Consequently, the only expression we have to specify is the 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tau_0)$ in equation analogous to eq. (29). To specify $\hat{\mathbf{M}}^{(x)}(\tau_0)$ at a point τ_0 of the ray, we again use the equation (43). The vectors $\mathbf{p}(\tau_0)$, $\boldsymbol{\mathcal{U}}(\tau_0)$ and $\boldsymbol{\eta}(\tau_0)$ are known; they can be obtained from ray tracing equations at τ_0. The unit basis vectors $\mathbf{e}_1(\tau_0)$ and $\mathbf{e}_2(\tau_0)$, necessary for the determination of vectors $\mathbf{f}_1(\tau_0)$ and $\mathbf{f}_2(\tau_0)$, must be unit, mutually perpendicular and perpendicular to the slowness vector $\mathbf{p}(\tau_0)$. Otherwise, they can be chosen arbitrarily. They also represent vector basis for the 2×2 matrix $\mathbf{M}^{(q)}(\tau_0)$ (with elements $\partial^2 T/\partial q^M \partial q^N$).

In this way, we have three alternative possibilities of computation of the paraxial travel time field and Gaussian beams in Cartesian coordinates.

1. We compute first the 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ in Cartesian coordinates. In this case, the DRT system consists of 6 equations. To compute the 6×6 ray propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ requires to solve the DRT system six times (i.e., 36 equations). We, however, remind the reader that the coefficients of the DRT system are evaluated only once so that the solution is fast. The 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tau)$ is then obtained automatically at any point of the ray. To apply formula analogous to (29), however, we need to know the 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tau_0)$ at the point $\tau = \tau_0$.

2. We perform the simplified dynamic ray tracing. The DRT system is the same as sub 1 and consists again of 6 equations. Solving this system four times (i.e., 24 equations), with specific initial conditions (33) and (34), we can determine the 4×4 ray propagator matrix in wavefront orthonormal coordinates, which is equivalent to the 4×4 ray propagator matrix in ray-centred coordinates. Given the matrix of second derivatives of the travel time field $\mathbf{M}^{(q)}(\tau_0)$ with respect to the ray-centred coordinates at the point $\tau = \tau_0$, we can use (29) and determine $\mathbf{M}^{(q)}(\tau)$ at any point of the ray Ω. The paraxial observation point R may be specified in Cartesian coordinates.

3. We compute first the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ in ray-centred coordinates, given by (25). The DRT system consists of four equations, and we have to solve it four times (i.e., 16 equations). At the required termination point of the ray Ω, we then determine the 3×3 matrix $\hat{\mathbf{M}}^{(x)}(\tau)$ using (43). The paraxial travel time and the Gaussian beam are then determined using (12) and (44). The same possibility applies to wavefront orthonormal coordinates.

The numerical efficiency of the above approaches has not yet been fully investigated and compared. For inhomogeneous generally anisotropic media, all approaches require to determine 21 second derivatives of the Hamiltonian $\mathcal{H}(x_i, p_j)$, namely $\partial^2\mathcal{H}/\partial x_i \partial x_j$, $\partial^2\mathcal{H}/\partial x_i \partial p_j$, $\partial^2\mathcal{H}/\partial p_i \partial p_j$, at any point of the ray Ω. In other aspects, however, the algorithms differ. The differences are mainly in the computation of the 6×6 ray-propagator matrix $\mathbf{\Pi}^{(x)}(\tau, \tau_0)$ and the computation of the 4×4 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$.

4.3 Properties of Gaussian beams

In Sections 4.1 and 4.2, we derived two expressions for Gaussian beams, concentrated close to the central ray, in inhomogeneous anisotropic layered media. The first of them, given by (40) with (41), is expressed fully in ray-centred coordinates. The expression is very simple, but has a serious disadvantage. It can be used only if the observation point R is specified in ray-centred coordinates. Consequently, we have to find the point R_Ω on the ray Ω, at which the plane containing the observation point R is tangent to the wavefront. The numerical procedure to determine the ray-centred coordinates q_1, q_2, q_3 of the observation point R is rather cumbersome. Consequently, the expressions (40) with (41) are not suitable in the summation of Gaussian beams at an à priori specified observation point R, as it would require to repeat the cumbersome procedure for any Gaussian beam used in the summation.

The second expression for the Gaussian beam, given by (45) with (46)–(48) is considerably more general and flexible, as the position of the observation point R may be specified in Cartesian coordinates. Moreover, we can use any point R_Ω situated on the ray Ω as the reference point in (45). Of course, it is desirable to consider the point R_Ω as close to the observation point as possible. Similarly as in the expression (40), we determine the 2×2 matrix $\mathbf{M}^{(q)}(R_\Omega)$ of second derivatives of the complex-valued travel-time field at point R_Ω. The 2×2 matrix $\mathbf{M}^{(q)}(R_\Omega)$ may be calculated alternatively by DRT in ray-centred coordinates, in wavefront orthonormal coordinates, or in simplified Cartesian coordinates. Which of these approaches is numerically most efficient is not yet quite clear and requires more detailed numerical studies. In any case, the DRT in global Cartesian coordinates, with the complete 6×6 ray-propagator matrix, is not necessary; the simplified DRT leading to the 4×4 ray propagator matrix is sufficient.

As soon as we determine the 2×2 matrix $\mathbf{M}^{(q)}(R_\Omega)$, the Gaussian beam at the required reference point R_Ω may be easily transformed to Cartesian coordinates, independently on how the 2×2 matrix $\mathbf{M}^{(q)}(R_\Omega)$ was calculated.

From physical point of view, the expression (45) has another advantage in comparison with the relation (40). The expression (40) is expressed in terms of coordinates q_1, q_2, related to the plane tangent to the wavefront at the point R_Ω on the central ray Ω. The expressions (45)–(48), however, are expressed in terms of basis vectors $\mathbf{f}_1, \mathbf{f}_2$, perpendicular to the ray Ω at R_Ω. The behaviour of a Gaussian beam is better understood if it is expressed in the plane perpendicular to the ray Ω than in the plane tangent to the wavefront.

Actually, equations (40) with (41) are a special case of (45)–(48) and can be simply obtained from them. Consider the observation point R situated in the plane tangent to the wavefront at R_Ω. Then we can express the position of the point R in ray-centred coordinates using the relation

$$\mathbf{x}(R) - \mathbf{x}(R_\Omega) = q_1\mathbf{e}_1 + q_2\mathbf{e}_2 \ . \tag{49}$$

Using (48) for $\tilde{\mathbf{f}}$, we obtain

$$\tilde{\mathbf{f}} = (q_1\mathbf{e}_1 + q_2\mathbf{e}_2)^T(\mathbf{f}_1, \mathbf{f}_2) = (q_1, q_2) = \mathbf{q}^T \ . \tag{50}$$

From (50), we obtain the Gaussian beam exponential factor, which controls the amplitude profile of the beam:

$$\exp[-\tfrac{1}{2}\omega\tilde{\mathbf{f}}\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)\tilde{\mathbf{f}}^T] = \exp[-\tfrac{1}{2}\omega\mathbf{q}^T\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)\mathbf{q}] \ . \tag{51}$$

Consider now the expression (46) for $\mathrm{Re}T(R, R_\Omega)$ in the plane tangent to the wavefront at R_Ω. As the slowness vector $\mathbf{p}$ is perpendicular to this plane at R_Ω, we obtain $\tilde{p} = 0$. Consequently, three terms in (46) containing $\tilde{p}$ vanish. Using eq. (50), the term $\frac{1}{2}\tilde{\mathbf{f}}\mathrm{Re}\mathbf{M}^{(q)}(R_\Omega)\tilde{\mathbf{f}}^T$ can be transformed into $\frac{1}{2}\mathbf{q}^T\mathrm{Re}\mathbf{M}^{(q)}(R_\Omega)\mathbf{q}$. Thus, equations (40)–(41)

for the Gaussian beam in the plane tangent to the wavefront at R_Ω, obtained in Section 3.3, follow also from equations (45)–(48). For this reason, we shall consider exclusively the expressions (45)–(48) in the following.

We now explain the meaning of individual factors in equations (45)–(48) from physical point of view. The most important factor in equation (45) is the exponential factor $\exp[-\omega \mathrm{Im} T(R, R_\Omega)]$, with $\mathrm{Im} T(R, R_\Omega)$ given by (47). This factor shows that the Gaussian beam is concentrated close to the ray Ω and that its amplitude profile in a plane perpendicular to $\boldsymbol{\mathcal{U}}(R_\Omega)$, i.e., perpendicular to the ray Ω, is Gaussian in any section containing R_Ω. Similarly, the amplitude profile in a plane tangent to the wavefront at R_Ω is Gaussian in any section containing R_Ω. This is the reason why the solutions (40)–(41) and (45)–(48) are called Gaussian beams.

The amplitude profile of the Gaussian beam in any section containing R_Ω is controlled by the 2×2 matrix $\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)$. As $\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)$ is symmetric and positive definite, it has two positive real-valued eigenvalues $M_1^{(q)I}(R_\Omega)$ and $M_2^{(q)I}(R_\Omega)$ at any point R_Ω of the ray Ω. With the increasing square of the distance from the ray Ω in the plane perpendicular to the ray Ω, the amplitudes decrease exponentially. The exponential decrease is frequency dependent, it is faster for higher frequencies and slower for lower frequencies. Quadratic curve $\frac{1}{2}\omega\tilde{\mathbf{f}}^T(R_\Omega)\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)\tilde{\mathbf{f}}(R_\Omega) = 1$ in the plane perpendicular to the ray Ω is usually called the spot ellipse for frequency ω. Spot ellipse in the plane perpendicular to the ray Ω is, of course, different from the spot ellipse in the plane tangent to the wavefront at R_Ω, which is specified by the quadratic curve $\frac{1}{2}\omega\mathbf{q}^T(R_\Omega)\mathrm{Im}\mathbf{M}^{(q)}(R_\Omega)\mathbf{q}(R_\Omega) = 1$. Along both spot ellipses, the amplitude of the Gaussian beam is constant.

Instead of the eigenvalues $M_1^{(q)I}(R_\Omega)$ and $M_2^{(q)I}(R_\Omega)$ of the 2×2 matrix $\mathrm{Im}\,\mathbf{M}^{(q)}(R_\Omega)$, we can also use the quantities $L_1(R_\Omega)$ and $L_2(R_\Omega)$, given by the relation

$$L_{1,2}(R_\Omega) = [\pi M_{1,2}^{(q)I}(R_\Omega)]^{-1/2} \ . \tag{52}$$

Quantities $L_1(R_\Omega)$ and $L_2(R_\Omega)$ represent the half-axes of the spot ellipse at R_Ω for frequency $f = 1$Hz (i.e., $\omega = 2\pi$). We call them the half-widths of the Gaussian beam.

The 2×2 matrix $\mathrm{Re}\mathbf{M}^{(q)}(R_\Omega)$ describes the geometric properties of the phase front of the Gaussian beam. Because $\mathrm{Re}\mathbf{M}^{(q)}(R_\Omega)$ is always symmetrical, its eigenvalues $M_1^{(q)R}(R_\Omega)$ and $M_2^{(q)R}(R_\Omega)$ are always real. Instead of $\mathrm{Re}\mathbf{M}^{(q)}(R_\Omega)$, we can introduce the 2×2 matrix $\mathbf{K}(R_\Omega)$ of the curvature of the phase front at R_Ω on the ray Ω by relation

$$\mathbf{K}(R_\Omega) = \mathcal{C}(R_\Omega)\mathrm{Re}\mathbf{M}^{(q)}(R_\Omega) \ , \tag{53}$$

where $\mathcal{C}(R_\Omega)$ is the phase velocity (the velocity in the direction of the slowness vector $\mathbf{p}(R_\Omega)$). Then the eigenvalues of $\mathbf{K}(R_\Omega)$ represent the principal curvatures of the phase front of the Gaussian beam at the point R_Ω on Ω.

The half-width of the Gaussian beam varies along the ray Ω. We can determine these variations from the expressions (52) and (29). Consequently, the Gaussian beams may be narrow in some regions of the ray, but broad in other regions. Similarly, the curvature of the phase front of the Gaussian beam varies along the ray Ω and may be determined using (53) and (29).

5 Concluding remarks

The derived expressions for the Gaussian beams in inhomogeneous anisotropic layered media are valid for anisotropy of arbitrary symmetry, specified by upto 21 density-normalized elastic moduli $a_{ijkl}(x_n)$, which are arbitrary functions of coordinates x_n. Of course, it is assumed that the general validity conditions of the ray method are satisfied to compute sufficiently accurate ray propagator matrices along the ray.

The basic quantity in the computation of Gaussian beams in inhomogeneous anisotropic layered media is the complex-valued 2×2 matrix $\mathbf{M}^{(q)}(\tau)$ of second derivatives of the travel-time field with respect to ray-centred coordinates, with elements $\partial^2 T/\partial q_N \partial q_M$. This matrix can be computed by dynamic ray tracing, in three alternative versions: a) by DRT in ray-centred coordinates q_1, q_2, q_3, b) by DRT in wavefront orthonormal coordinates y_1, y_2, y_3, c) by simplified DRT in Cartesian coordinates. The decision, which of these three methods is numerically most efficient, would require extensive numerical testing. Once the 2×2 matrix $\mathbf{M}^{(q)}(\tau)$ is known along the central ray Ω, the flexible and numerically efficient expressions (45)–(48) for Gaussian beam can be used.

As the model of an inhomogeneous anisotropic layered medium under consideration is very general, and as the ray-propagator matrix is used in the algorithm, the relevant procedures are rather involved. They may be, however, simplified in many special cases. Such simplifications lead to more efficient algorithms. The most decisive role is played by the simplifications of ray-tracing computations and of the computation of the ray propagator matrix.

In the following, we shall list several such possible simplifications.

a) Considerable simplifications can be obtained for higher anisotropic symmetries, for example for the transversely isotropic (TI) or orthorhombic media.

b) Further simplification can be obtained for weakly anisotropic media. This is true particularly for P waves. For S waves, their coupling in weakly anisotropic media must be taken into account. In this case, Gaussian beams could be constructed along so-called common rays. It may be useful to use so-called first-order ray tracing (Pšenčík and Farra, 2005,2007; Farra and Pšenčík, 2008, 2009).

c) For anisotropy symmetries with spatially varying elements of symmetry, the ray-tracing and dynamic ray-tracing computations in Cartesian coordinates are quite cumbersome and even inaccurate. Iversen and Pšenčík (2007, 2008) proposed procedure based on the evaluation of quantities important for the ray tracing and dynamic ray tracing in a coordinate system connected with the symmetry elements of the considered medium. The procedure conserves the symmetry of the studied medium throughout the model and increases considerably efficiency (computer-time and memory savings).

d) Considerably more efficient algorithms for ray tracing and ray propagator matrix computations are obtained for factorized inhomogeneous anisotropic media, in which all density normalized elastic moduli vary spatially in the same way. The simplest factorized inhomogeneous anisotropic media are media, in which the gradient (e.g., the vertical gradient) of all density normalized elastic moduli is the same in the whole region under interest. See more details in Červený (1989), Shearer and Chapman (1989).

e) A simple and numerically very efficient algorithm would be obtained for a medium composed of homogeneous anisotropic layers (blocks), or composed of different inhomogeneous factorized anisotropic layers (blocks).

f) Instead of the Hamiltonian $\mathcal{H}(x_i, p_j)$, we can consider the reduced Hamiltonian $\mathcal{H}^R(x_I, p_J)$. The reduced Hamiltonians are, however, known for transversely isotropic media and isotropic media only.. Both the ray tracing and dynamic ray tracing simplify in this case. Mostly, the horizontal components of the slowness vector p_1 and p_2 are computed by ray tracing, and the vertical component p_3 of the slowness vector must be determined in terms of p_1 and p_2. See Červený, Molotkov and Pšenčík (1977, section 5.5.2), Červený (2001, section 4.2.4/1).

g) Instead of general 3-D configurations, considered in this text, we can sometimes consider 2-D configurations, which considerably simplifies the procedures. For inhomogeneous media of general anisotropy, however, the 2-D configurations do not play such an important role as for isotropic inhomogeneous media. It is because of a different direction of the ray-velocity vector, the slowness vector and the polarization vector, due to which the wave propagation in inhomogeneous anisotropic media is generally three-dimensional. Only in the planes of symmetry of transversely isotropic and orthorhombic media such a situation may play an important role.

The simplifications of the general procedure given in this text for situations outlined in this section will be described in a greater detail elsewhere.

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Appendix A
Ray-tracing system in inhomogeneous anisotropic media

We consider the eikonal equation for inhomogeneous anisotropic media, given in the Hamiltonian form $\mathcal{H}(x_i, p_j) = 0$. The Hamiltonian $\mathcal{H}(x_i, p_j)$ is defined by the relation

$$\mathcal{H}(x_i, p_j) = \tfrac{1}{2}(G_m(x_i, p_j) - 1) \ , \qquad (A-1)$$

where G_m, $m = 1, 2, 3$, is a selected eigenvalue of the Christoffel matrix $\Gamma_{ik}(x, p) = a_{ijkl} p_j p_l$. The ray tracing system is then given by the system of six nonlinear ordinary differential equations of the first order,

$$\frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \frac{\partial \mathcal{H}}{\partial p_i} \ , \quad \frac{\mathrm{d}p_i}{\mathrm{d}\tau} = -\frac{\partial \mathcal{H}}{\partial x_i} \ . \qquad (A-2)$$

Here the parameter τ along the ray represents the travel time. The right-hand sides of the ray tracing system (A-2) represent components $\mathcal{U}_i = \partial\mathcal{H}/\partial p_i$ of the ray velocity vector $\boldsymbol{\mathcal{U}}$, and $\eta_i = -\partial\mathcal{H}/\partial x_i$ of the vector $\boldsymbol{\eta}$. They can be computed using the equations

$$\frac{\partial \mathcal{H}}{\partial p_i} = \mathcal{U}_i = a_{ijkl} p_l g_j^{(m)} g_k^{(m)} \ , \quad -\frac{\partial \mathcal{H}}{\partial x_i} = \eta_i = -\tfrac{1}{2} \frac{\partial a_{jkln}}{\partial x_i} p_k p_n g_j^{(m)} g_l^{(m)} \ . \qquad (A-3)$$

(no summation over m). The vector $\mathbf{g}^{(m)}$, $m = 1, 2, 3$, denotes the unit eigenvector of the Christoffel matrix corresponding to the eigenvalue G_m of the wave under consideration (P, S1, S2).

The equations (A-3) contain the eigenvector $\mathbf{g}^{(m)}$ of the Christoffel matrix. Alternatively, we can use other expressions for $\partial\mathcal{H}/\partial p_i$ and $-\partial\mathcal{H}/\partial x_i$, which do not contain the eigenvector $\mathbf{g}^{(m)}$ explicitly. These expressions are, however, algebraically more complicated. They read

$$\frac{\partial \mathcal{H}}{\partial p_i} = \mathcal{U}_i = a_{ijkl} p_l D_{jk}/D_{ss} \ , \quad -\frac{\partial \mathcal{H}}{\partial x_i} = \eta_i = -\frac{1}{2} \frac{\partial a_{jkln}}{\partial x_i} p_k p_n D_{jl}/D_{ss} \ . \qquad (A-4)$$

Here

$$D_{jk}/D_{ss} = g_j^{(m)} g_k^{(m)} = \tfrac{1}{2} \epsilon_{ikl} \epsilon_{jrs} (\Gamma_{kr} - \delta_{kr})(\Gamma_{ls} - \delta_{ls}) \ . \qquad (A-5)$$

The symbol ϵ_{ijk} represents the Levi-Civita symbol ($\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$, $\epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1$, $\epsilon_{ijk} = 0$ otherwise).

Anisotropic ray tracing system (A-2), with (A-3) or (A-4), can be used quite universally for P waves, including P waves in heterogeneous isotropic and weakly anisotropic media. For S waves, however, the situation is more complicated. Ray tracing fails in the vicinity of S-wave singularities, where the two eigenvalues corresponding to S waves are equal or close to each other. Ray tracing for S waves may fail globally in very weakly anisotropic media, and fails in isotropic media. Remember that two eigenvalues of S waves are equal in isotropic media. These problems can be removed if the coupling ray theory for shear waves or its various modifications are used (Kravtsov, 1968; Coates and Chapman, 1990; Bakker, 2002; Klimeš, 2006b; Farra and Pšenčík, 2009).

The ray method was first proposed for the computation of high-frequency seismic wave fields in inhomogeneous anisotropic media by Babich (1961). Equations (A-4) for ray tracing in inhomogeneous anisotropic media were derived by Červený (1972). For more details on ray tracing in inhomogeneous anisotropic media, see Červený (2001, chap. 3.6). The computer program for ray tracing in inhomogeneous anisotropic layered structure based on the above-mentioned formulae is the computer package ANRAY (Gajewski and Pšenčík, 1987,1990). The package ANRAY is freely available on the web pages of the consortium SW3D (http://sw3d.mff.cuni.cz/).

Let us now assume that a ray hits a curved structural interface. In the framework of the zero-order ray method, the reflection/transmission problem in the vicinity of the point of incidence is considered as the problem of incidence of a plane wave at a plane interface separating two homogeneous media. Three reflected and three transmitted waves (P, S1, S2) are generated at the point of incidence; some of them may be inhomogeneous. We denote any of generated waves by the superscript (m). The slowness vector of this, reflected or transmitted, wave is given by the relation

$$\mathbf{p}^{(m)} = \sigma \mathbf{n} + \mathbf{p}^{\Sigma} \ . \qquad (A-6)$$

Here $\mathbf{n}$ is the unit vector perpendicular to the interface at the point of incidence, with arbitrary orientation. The symbol $\mathbf{p}^{\Sigma}$ denotes the tangential component to the interface of the slowness vector of the incident wave. The component $\mathbf{p}^{\Sigma}$ is the same for incident and all generated waves. This equality is just another expression of the Snell law. The projection of the slowness vector to the normal $\mathbf{n}$, σ, is a root of the algebraic equation of the sixth degree:

$$\det[a_{ijkl}(\sigma n_j + p_j^{\Sigma})(\sigma n_l + p_l^{\Sigma}) - \delta_{ij}] = 0 \ . \qquad (A-7)$$

For reflected waves, we use the same elastic moduli a_{ijkl} as for incident waves. For transmitted waves, we use a_{ijkl} corresponding to the halfspace on the other side of the interface.

Equation (A-7) gives six solutions for each halfspace. The physical solutions corresponding to the three reflected and three transmitted waves are selected from them according to the direction of the relevant ray-velocity vector $\boldsymbol{\mathcal{U}}$ (for real-valued roots) and according to the radiation conditions (for complex-valued roots).

For more details, see Červený (2001, section 2.3.3).

Appendix B
Dynamic ray tracing systems in inhomogeneous anisotropic media

The dynamic ray tracing consists in the solution of a system of linear ordinary differential equations of the first order along the ray Ω. The system may be solved together with the ray tracing, or along an already known ray Ω. Here we present three versions of the dynamic ray tracing system, namely the dynamic ray tracing system in global Cartesian coordinates, in ray-centred coordinates and in wavefront orthonormal coordinates. Each of these systems has its advantages and disadvantages.

Dynamic ray tracing in global Cartesian coordinates consists of six equations for $Q_{ij}^{(x)} = \partial x_i / \partial \gamma_j$, and $P_{ij}^{(x)} = \partial p_i / \partial \gamma_j$ with $i = 1, 2, 3$ and j fixed. The complete 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ can be obtained by solving the DRT system three times with proper initial conditions. The dynamic ray tracing system in Cartesian coordinates can be simply derived by differentiating the ray tracing equations (A-2) with respect to γ_j. It reads:

$$\frac{\mathrm{d}Q^{(x)}_{ij}}{\mathrm{d}\tau} = A^{(x)}_{im}Q^{(x)}_{mj} + B^{(x)}_{im}P^{(x)}_{mj} \ ,$$

$$\frac{\mathrm{d}P^{(x)}_{ij}}{\mathrm{d}\tau} = -C^{(x)}_{im}Q^{(x)}_{mj} - D_{im}P^{(x)}_{mj} \ . \qquad (B-1)$$

Here

$$A^{(x)}_{im} = \frac{\partial^2\mathcal{H}}{\partial p_i \partial x_m} \ , \quad B^{(x)}_{im} = \frac{\partial^2\mathcal{H}}{\partial p_i \partial p_m} \ ,$$

$$C^{(x)}_{im} = \frac{\partial^2\mathcal{H}}{\partial x_i \partial x_m} \ , \quad D^{(x)}_{im} = \frac{\partial^2\mathcal{H}}{\partial x_i \partial p_m} \ . \qquad (B-2)$$

Note that $D^{(x)}_{im} = A^{(x)}_{mi}$.

The DRT system in Cartesian coordinates for inhomogeneous anisotropic media was first derived by Červený (1972), with the purpose to compute geometrical spreading and ray amplitudes.Its other applications and the algorithms for the determination of the 3×3 matrices $\hat{\mathbf{A}}^{(x)}$, $\hat{\mathbf{B}}^{(x)}$, $\hat{\mathbf{C}}^{(x)}$ and $\hat{\mathbf{D}}^{(x)}$ are discussed in Červený (2001, sec. 4.14.1). See also Gajewski and Pšenčík (1990). The DRT system in the form (B-1), (B-2) is used in the program package ANRAY (http://sw3d.mff.cuni.cz/).

Dynamic ray tracing in ray-centred coordinates consists of four equations for $Q^{(q)}_{IJ} = \partial q_I/\partial\gamma_J$ and $P^{(q)}_{IJ} = \partial p^{(q)}_I/\partial\gamma_J$, with $I = 1, 2$ and J fixed. The complete 2×2 matrices $\mathbf{Q}^{(q)}$ and $\mathbf{P}^{(q)}$ are obtained by solving the DRT system two times, with proper initial conditions. The symbol $p^{(q)}_I$ denotes the I-th ray-centred component of the slowness vector. The system reads:

$$\frac{\mathrm{d}Q^{(q)}_{IM}}{\mathrm{d}\tau} = A^{(q)}_{IJ}Q^{(q)}_{JM} + B^{(q)}_{IJ}P^{(q)}_{JM} \ ,$$

$$\frac{\mathrm{d}P^{(q)}_{IM}}{\mathrm{d}\tau} = -C^{(q)}_{IJ}Q^{(q)}_{JM} - D^{(q)}_{IJ}P^{(q)}_{JM} \ . \qquad (B-3)$$

Here the 2×2 matrices $\mathbf{A}^{(q)}$, $\mathbf{B}^{(q)}$, $\mathbf{C}^{(q)}$ and $\mathbf{D}^{(q)}$, can be calculated from 3×3 matrices $\hat{\mathbf{A}}^{(x)}$, $\hat{\mathbf{B}}^{(x)}$, $\hat{\mathbf{C}}^{(x)}$ and $\hat{\mathbf{D}}^{(x)}$, given in (B-2), as follows:

$$\mathbf{A}^{(q)} = \mathbf{f}^T\hat{\mathbf{A}}^{(x)}\mathbf{e} + \mathbf{d} \ , \quad \mathbf{B}^{(q)} = \mathbf{f}^T\hat{\mathbf{B}}^{(x)}\mathbf{f} \ ,$$

$$\mathbf{C}^{(q)} = \mathbf{e}^T(\hat{\mathbf{C}}^{(x)} - \boldsymbol{\eta}\boldsymbol{\eta}^T)\mathbf{e} \ , \quad \mathbf{D}^{(q)} = \mathbf{e}^T\hat{\mathbf{D}}^{(x)}\mathbf{f} + \mathbf{d}^T \ . \qquad (B-4)$$

The 3×2 matrix $\mathbf{e}$ is composed of two unit basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ tangent to the wavefront: $\mathbf{e} = (\mathbf{e}_1, \mathbf{e}_2)$. Using $\mathbf{e}_1$ and $\mathbf{e}_2$, we can also compute the 3×2 matrix $\mathbf{f} = (\mathbf{f}_1, \mathbf{f}_2)$ composed of vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ perpendicular to the ray:

$$\mathbf{f}_1 = \frac{\mathbf{e}_2 \times \boldsymbol{\mathcal{U}}}{\boldsymbol{\mathcal{U}}^T(\mathbf{e}_1 \times \mathbf{e}_2)} \ , \quad \mathbf{f}_2 = \frac{\boldsymbol{\mathcal{U}} \times \mathbf{e}_1}{\boldsymbol{\mathcal{U}}^T(\mathbf{e}_1 \times \mathbf{e}_2)} \ . \qquad (B-5)$$

Finally, $\mathbf{d} = \mathbf{f}^T d\mathbf{e}/d\tau$, where the derivative $\mathrm{d}\mathbf{e}/\mathrm{d}\tau$ is given by (14).

The dynamic ray tracing system in ray-centred coordinates for inhomogeneous anisotropic media was first derived by Kendall et al. (1992) and by Klimeš (1994, 2006a). See also Červený (2001).

Dynamic ray tracing system in wavefront orthonormal coordinates consists of four equations for $Q^{(y)}_{IJ} = \partial y_I/\partial\gamma_J$ and $P^{(y)}_{IJ} = \partial p^{(y)}_I/\partial\gamma_J$, $I = 1,2$, J fixed. The complete 2×2 matrices $\mathbf{Q}^{(y)}$ and $\mathbf{P}^{(y)}$ are obtained by solving the DRT system two times, with proper initial conditions. The symbol $p^{(y)}_I$ denotes the I-th wavefront orthonormal component of the slowness vector. The dynamic ray tracing system reads (see Bakker, 1996, Červený, 2001):

$$\frac{\mathrm{d}Q^{(y)}_{IM}}{\mathrm{d}\tau} = A^{(y)}_{IJ}Q^{(y)}_{JM} + B^{(y)}_{IJ}P^{(y)}_{JM} \ ,$$

$$\frac{\mathrm{d}P^{(y)}_{IM}}{\mathrm{d}\tau} = -C^{(y)}_{IJ}Q^{(y)}_{JM} - D^{(y)}_{IJ}P^{(y)}_{JM} \ . \qquad (B-6)$$

Here the 2×2 matrices $\mathbf{A}^{(y)}$, $\mathbf{B}^{(y)}$, $\mathbf{C}^{(y)}$ and $\mathbf{D}^{(y)}$ can be calculated from the 3×3 matrices $\hat{\mathbf{A}}^{(x)}$, $\hat{\mathbf{B}}^{(x)}$, $\hat{\mathbf{C}}^{(x)}$ and $\hat{\mathbf{D}}^{(x)}$, given by (B-2), as follows:

$$\mathbf{A}^{(y)} = \mathbf{e}^T(\mathbf{A}^{(x)} + \boldsymbol{\mathcal{U}}\boldsymbol{\eta}^T)\mathbf{e} \ , \quad \mathbf{B}^{(y)} = \mathbf{e}^T(\mathbf{B}^{(x)} - \boldsymbol{\mathcal{U}}\boldsymbol{\mathcal{U}}^T)\mathbf{e} \ ,$$

$$\mathbf{C}^{(y)} = \mathbf{e}^T(\mathbf{C}^{(x)} - \boldsymbol{\eta}\boldsymbol{\eta}^T)\mathbf{e} \ , \quad \mathbf{D}^{(y)} = \mathbf{e}^T(\mathbf{D}^{(x)} + \boldsymbol{\eta}\boldsymbol{\mathcal{U}}^T)\mathbf{e} \ . \qquad (B-7)$$

All vectors in (B-7) are expressed in Cartesian coordinates. It was shown in Červený (2007) that the dynamic ray tracing system in ray-centred coordinates, (B-3) with (B-4), is fully equivalent to the dynamic ray tracing system in wavefront orthonormal coordinates, (B-6) with (B-7).

Appendix C
Properties of ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$

In this appendix, we consider a 4×4 ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ in ray-centred coordinates. We describe its important properties which can be conveniently used in paraxial ray theory and in the theory of Gaussian beams. The properties of the 6×6 ray propagator matrix in Cartesian coordinates are exactly the same, only all matrices would be 6×6.

The most important property of the ray propagator matrix is its symplecticity. This means that it satisfies the following matrix relation:

$$\mathbf{\Pi}^T(\tau,\tau_0)\mathbf{J}\mathbf{\Pi}(\tau,\tau_0) = \mathbf{J} \ , \qquad (C-1)$$

where $\mathbf{J}$ is the 4×4 matrix

$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix} \ . \qquad (C-2)$$

In (C-2), $\mathbf{I}$ is the 2×2 identity matrix and $\mathbf{0}$ is the 2×2 null matrix. The symplecticity of $\mathbf{\Pi}(\tau,\tau_0)$ has several important and useful consequences:

a) The matrix $\mathbf{\Pi}(\tau,\tau_0)$ satisfies the Liouvillé's theorem

$$\det\mathbf{\Pi}(\tau,\tau_0) = 1 \ . \qquad (C-3)$$

Equation (C-3) is satisfied for any τ. Consequently, $\mathbf{\Pi}(\tau,\tau_0)$ is regular along the whole ray Ω.

b) The matrix $\mathbf{\Pi}(\tau,\tau_0)$ satisfies the chain rule:

$$\mathbf{\Pi}(\tau,\tau_0)=\mathbf{\Pi}(\tau,\tau_1)\mathbf{\Pi}(\tau_1,\tau_0)\ . \qquad (C-4)$$

The point corresponding to τ_1 may be an arbitrary point of the ray Ω, not necessarily between τ_0 and τ. The chain rule (C-4) can be extended to an arbitrary number of points τ_1, τ_2, τ_3, ... τ_n along the ray Ω.

c) The inverse propagator matrix $\mathbf{\Pi}(\tau_0,\tau)=\mathbf{\Pi}^{-1}(\tau,\tau_0)$ of $\mathbf{\Pi}(\tau,\tau_0)$ is always regular and is given by the relation

$$\mathbf{\Pi}^{-1}(\tau,\tau_0)=\begin{pmatrix} \mathbf{P}_2^T(\tau,\tau_0) & -\mathbf{Q}_2^T(\tau,\tau_0) \\ -\mathbf{P}_1^T(\tau,\tau_0) & \mathbf{Q}_1^T(\tau,\tau_0) \end{pmatrix}\ . \qquad (C-5)$$

d) The symplecticity relation (C-1) leads to four 2×2 matrix relations, which are invariant with respect to τ varying along the ray Ω:

$$\begin{array}{ll} \mathbf{Q}_1^T\mathbf{P}_1-\mathbf{P}_1^T\mathbf{Q}_1=\mathbf{0}\ , & \mathbf{P}_2^T\mathbf{Q}_1-\mathbf{Q}_2^T\mathbf{P}_1=\mathbf{I}\ , \\ \mathbf{Q}_2^T\mathbf{P}_2-\mathbf{P}_2^T\mathbf{Q}_2=\mathbf{0}\ , & \mathbf{Q}_1^T\mathbf{P}_2-\mathbf{P}_1^T\mathbf{Q}_2=\mathbf{I}\ . \end{array} \qquad (C-6)$$

e) The matrix $\mathbf{\Pi}(\tau,\tau_0)$ can be constructed even if the ray Ω is reflected/transmitted at a structural interface between τ_0 and τ. Let us introduce the travel times τ^{inc} and τ^R corresponding to the point of incidence and to the point of reflection/transmission, respectively. Of course, $\tau^R=\tau^{inc}$, but the slowness vectors $\mathbf{p}$, ray-velocity vectors $\boldsymbol{\mathcal{U}}$, etc. are different for τ^{inc} and τ^R. The ray propagator matrix $\mathbf{\Pi}(\tau,\tau_0)$ then reads:

$$\mathbf{\Pi}(\tau,\tau_0)=\mathbf{\Pi}(\tau,\tau^R)\mathbf{\Pi}(\tau^R,\tau^{inc})\mathbf{\Pi}(\tau^{inc},\tau_0)\ . \qquad (C-7)$$

The 2×2 matrix $\mathbf{\Pi}(\tau^R,\tau^{inc})$ is usually called the *interface propagator matrix*. The expressions for the interface propagator matrix are derived and discussed in detail in Moser (2004), Červený and Moser (2007) and Moser and Červený (2007), both in Cartesian and ray-centred coordinates. Thus, the ray propagator matrix in a layered medium is obtained by considering the interface propagator matrix at every point of incidence of the ray at a structural interface.

The properties of ray-propagator matrices are well-known even in other branches of seismology, where propagator matrices are used. Let us name here, for example, the computation of wave fields in 1-D vertically inhomogeneous media. For classical references, see Gilbert and Backus (1966), Ursin (1983), Kennett (1983).

Appendix D
Dynamic ray tracing with complex-valued initial conditions

Let us choose the initial conditions $\mathbf{Q}(\tau_0)$ and $\mathbf{P}(\tau_0)$ of the dynamic ray tracing system in ray-centered coordinates complex valued:

$$\mathbf{Q}(\tau_0)=\mathbf{A}\ , \qquad \mathbf{P}(\tau_0)=\mathbf{M}_0\mathbf{A}\ . \qquad (D-1)$$

Here $\mathbf{A}$ is an arbitrary real-valued 2×2 matrix, different from the null matrix. The 2×2 matrix $\mathbf{M}_0$ is a complex-valued matrix satisfying the existence conditions of Gaussian beams. Then the matrix of second derivatives of the travel-time field with respect to ray-centred coordinates $\mathbf{M}(\tau_0)$ at the point $\tau = \tau_0$ equals $\mathbf{M}(\tau_0) = \mathbf{P}(\tau_0)\mathbf{Q}^{-1}(\tau_0) = \mathbf{M}_0\mathbf{A}\mathbf{A}^{-1} = \mathbf{M}_0$.

We can insert the intial conditions (D-1) into eq.(28) and obtain $\mathbf{Q}(\tau)$ and $\mathbf{P}(\tau)$. From this and (D-1) we get:

$$\mathbf{M}(\tau) = \mathbf{P}(\tau)\mathbf{Q}^{-1}(\tau) \qquad [\det\mathbf{Q}(\tau_0)/\det\mathbf{Q}(\tau)]^{1/2} = [\det\mathbf{A}/\det\mathbf{Q}(\tau)]^{1/2} \ . \qquad (D-2)$$

The results in (D-2) were obtained by using the ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$, see (28). It is possible to obtain exactly the same results by solving directly the DRT system with complex-valued initial conditions (D-1). In such a case, even the transformation relation (43) between $\mathbf{M}^{(x)}$ and $\mathbf{M}^{(q)}$ can be used.

The latter approach has been broadly used in the Gaussian beam migration in isotropic media, see Hill (1990, 2001), Gray (2005), Gray and Bleistein (2009). Matrix $\mathbf{M}_0$ has been mostly specified as purely imaginary, implying plane wavefront at $\tau = \tau_0$, with $\mathbf{A}$ controlling the initial halfwidth of the beam. Here we have shown that a similar approach can be used even in anisotropic media.

The advantage of the use of the ray-propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ is possibility to specify the complex-valued $\mathbf{M}_0$ at an arbitrary point of the ray Ω and to generate quantities (D-2) for varying specifications of $\mathbf{M}_0$ without repeating the solution of the dynamic ray tracing system.

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