

Seismic ray theory

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Summary

In this paper, the main principles of seismic ray theory for isotropic and anisotropic inhomogeneous media with curved structural interfaces are reviewed. Some extensions and modifications of seismic ray theory are also briefly mentioned.

Introduction

The ray theory belongs to the methods most frequently used in seismology and seismic exploration for forward and inverse modelling of high-frequency seismic body waves. In smoothly varying layered media, it can provide useful approximate solutions of satisfactory accuracy. Starting from an intuitive description of the propagation of seismic waves along special trajectories - rays, it has developed into a highly sophisticated method.

The ray method has its advantages and disadvantages. The basic advantage is its applicability to complex, isotropic and anisotropic, laterally varying layered media and its numerical efficiency in such computations. It provides a physical insight into the wave propagation process by separating the wavefield into individual elementary waves and by allowing their identification. In addition, it makes possible to track the paths in the medium along which energy propagates, an aspect very important in tomography. The ray method also represents an important basis for other related, more sophisticated methods, such as the Gaussian beam summation method, the paraxial ray method, the Maslov method, etc. The ray method also has some limitations. As mentioned above, it is approximate. It is applicable only to smooth media, in which the characteristic dimensions of inhomogeneities are considerably larger than the prevailing wavelength of the considered waves. The ray method can yield distorted results and may even fail in some special regions called *singular regions*.

The seismic ray method owes a lot to optics and radiophysics. Although the techniques used in different branches of physics are very similar, there are some substantial differences. The ray method in seismology is usually applied to more complicated structures than in optics or radiophysics. There are also different numbers and types of waves considered in different branches of physics.

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The first seismological applications date back to the end of the 19th century. Then, only *kinematics*, specifically travel times, were used. Probably the first attempts to use also *dynamics* (amplitudes and waveforms) were made by Sir H. Jeffreys. The ray series solutions of elastodynamic equations were first suggested by Babich (1956) and Karal and Keller (1959) for inhomogeneous isotropic media, and by Babich (1961) for inhomogeneous anisotropic media.

The Earth's interior is anisotropic or weakly anisotropic in some of its parts. Seismic anisotropy and its effects on wave propagation play an important role in contemporary seismology and seismic exploration. Consequently, it has also been necessary to develop the ray theory for anisotropic media. It is important to emphasize that, for S waves, the ray theory for weakly anisotropic media does not yield the ray theory for isotropic media in the zero anisotropy limit. For this reason, we describe systematically the ray theory for anisotropic media and also present corresponding formulae for isotropic media, and explain the differences between both of them.

S waves require generally a special attention. Well understood phenomenon is propagation of separate shear waves in anisotropic media. Less understood and an underestimated phenomenon is shear-wave coupling, which occurs in weakly anisotropic media or in vicinities of shear-wave singularities. In such regions, standard ray theories for anisotropic as well as isotropic media do not work properly. Therefore, we also briefly describe the coupling ray theory for S waves, which fills the gap between ray theories for isotropic and anisotropic media.

We give here neither a detailed derivation of ray-theoretical expressions nor a relevant systematic bibliography. This would extend the text considerably. We refer, however, to several textbooks, in which the ray theory is treated in a considerably greater detail (Červený et al., 1977; Kravtsov and Orlov, 1990; Červený, 2001; Chapman, 2004). The reader may also find useful information in several review papers devoted to seismic ray theory and its various aspects (Červený et al., 1988; Virieux, 1996; Chapman, 2002; Červený et al., 2007). Examples of computations based on the ray theory can be found, for example, in Červený et al. (1977), Gjøystdal et al. (2002). Here we refer only to papers, in which the relevant methods and procedures were first proposed, and/or which give a useful more recent treatment of the subject.

We use the following notation. We denote Cartesian coordinates x_i and time t . The dots above letters denote partial derivatives with respect to time ($\ddot{u}_i = \partial^2 u_i / \partial t^2$) and the index following the comma in the subscript indicates the partial derivative with respect to the relevant Cartesian coordinate ($u_{i,j} = \partial u_i / \partial x_j$). We consider high-frequency time-harmonic seismic body waves, with the exponential factor $\exp(-i\omega t)$, where ω is fixed, positive, real-valued circular frequency. The lower-case Roman indices take the values 1, 2, 3, the upper-case indices 1, 2. Hats over bold symbols indicate 3×3 matrices, bold symbols without hats denote 2×2 matrices. The Einstein summation convention over repeating Roman indices is used, with exception of indices in parentheses.

Basic equations of the seismic ray method

For smoothly varying elastic media, the source-free *equation of motion* reads

$$\tau_{ij,j} = \rho \ddot{u}_i . \quad (1)$$

Here $\tau_{ij}(x_n, t)$, and $u_i(x_n, t)$ are Cartesian components of stress tensor and displacement vector, respectively. In anisotropic media, the stress tensor τ_{ij} and the infinitesimal strain tensor $e_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ are related by Hooke's law:

$$\tau_{ij} = c_{ijkl}e_{kl} = c_{ijkl}\partial u_k/\partial x_l . \quad (2)$$

$c_{ijkl}(x_n)$ is a tensor of elastic moduli (stiffness tensor), satisfying symmetry relations $c_{ijkl} = c_{jikl} = c_{ijlk} = c_{klij}$. There are, at the most, 21 independent elastic moduli. Inserting eq.(2) into eq.(1), we get the *elastodynamic equation*

$$(c_{ijkl}u_{k,l})_{,j} = \rho \ddot{u}_i . \quad (3)$$

In the seismic ray method, high-frequency seismic body waves propagating in smoothly varying, isotropic or anisotropic, media are studied. The formal ray series solution of the elastodynamic equation (3) for the displacement vector $\mathbf{u}(x_n, t)$ is sought in the form of an asymptotic series in inverse powers of circular frequency ω ,

$$\mathbf{u}(x_n, t) = \exp[-i\omega(t - T(x_n))] \left[\mathbf{U}^{(0)}(x_n) + \frac{\mathbf{U}^{(1)}(x_n)}{(-i\omega)} + \frac{\mathbf{U}^{(2)}(x_n)}{(-i\omega)^2} + \dots \right] . \quad (4)$$

Here $T(x_n)$ is the real-valued travel time, $\mathbf{U}^{(k)}$, $k = 0, 1, 2, \dots$ are complex-valued *vectorial amplitude coefficients*. Surfaces $T(x_i) = \text{const.}$ are called *wavefronts*. In perfectly elastic media, functions $T(x_n)$, and $\mathbf{U}^{(k)}(x_n)$ are frequency independent. This is the great advantage of the ray method that it allows one to work with frequency-independent quantities.

Also other forms of the ray series have been used in the seismic ray method. For example, Chapman (2004) developed the seismic ray method using the ray series for particle velocity and traction. Such a formal ray series has certain advantages with respect to (4). Here, however, we consider systematically the traditional ray series (4) for the displacement vector.

Inserting (4) into elastodynamic equation (3), we obtain a series in inverse powers of ω , which equals zero. Consequently, the coefficients of the individual powers of ω must also equal zero. This yields a system of equations called the basic recurrence system of equations of the ray method. This system can be used to determine the eikonal equations for travel times $T(x_n)$ and, successively the equations for the amplitude coefficients $\mathbf{U}^{(0)}(x_n)$, $\mathbf{U}^{(1)}(x_n)$, $\mathbf{U}^{(2)}(x_n)$, The equations for $\mathbf{U}^{(k)}(x_n)$ yield, among others, transport equations. For a detailed derivation of the basic system of equations of the ray method see Červený (2001, Sec. 5.7).

The vectorial amplitude coefficients $\mathbf{U}^{(k)}(x_n)$, $k = 1, 2, \dots$, can be expressed as a sum of the *principal component* and *additional component*. The principal component of $\mathbf{U}^{(k)}(x_n)$

is the projection of $\mathbf{U}^{(k)}(x_n)$ into the unit vector parallel to the zero-order amplitude coefficient $\mathbf{U}^{(0)}(x_n)$, the additional component of $\mathbf{U}^{(k)}(x_n)$ is the remaining part of $\mathbf{U}^{(k)}(x_n)$. In this way, the additional component of the zero-order amplitude coefficient $\mathbf{U}^{(0)}(x_n)$ is zero. The complexity of the equations for higher-order amplitude coefficients $\mathbf{U}^{(k)}$ increases rapidly with increasing k . Moreover, the higher-order amplitude coefficients are inaccurate and unstable, as they are very sensitive to fine details of the medium. The instability of the amplitude coefficients increases with increasing k . For these reasons, only the zero-order coefficient $\mathbf{U}^{(0)}(x_n)$, at the most, with the additional component of $\mathbf{U}^{(1)}(x_n)$, has been used in seismological applications. In the following, we shall concentrate on the zero-order ray approximation only.

The zero-order approximation of the ray method reads:

$$\mathbf{u}(x_n, t) = \mathbf{U}(x_n) \exp[-i\omega(t - T(x_n))] . \quad (5)$$

In (5), we have dropped the superscript (0) of $\mathbf{U}(x_n)$. We call $\mathbf{U}(x_n)$ the complex-valued *vectorial amplitude*. In smooth, laterally varying media, containing smooth structural interfaces, the zero-order approximation (5) of the ray method usually offers sufficiently accurate results, particularly for travel time $T(x_n)$. However, if the medium under consideration becomes more and more complex (less smooth), vectorial amplitude $\mathbf{U}(x_n)$ becomes less accurate. In structures exceeding a certain degree of complexity, the ray method may yield inaccurate results or even fail.

The first equation of the basic system of equations of the ray method reads:

$$(\Gamma_{ik} - \delta_{ik})U_k = 0 , \quad i = 1, 2, 3 . \quad (6)$$

Here $\mathbf{\Gamma}$ is the 3×3 *generalized Christoffel matrix* with elements given by the relation:

$$\Gamma_{ik} = a_{ijkl}p_jp_l . \quad (7)$$

In (7), p_i are the Cartesian components of the slowness vector \mathbf{p} ,

$$p_i = \partial T / \partial x_i \quad (8)$$

and $a_{ijkl} = c_{ijkl} / \rho$ are density-normalized elastic moduli. Note that the classical Christoffel matrix, with elements $a_{ijkl}n_jn_l$, contains components of the real-valued unit vector \mathbf{n} (perpendicular to the wavefront) instead of \mathbf{p} . For this reason, we call (7) the “generalized” Christoffel matrix. The relation between p_i and n_i is $p_i = n_i / \mathcal{C}$, where \mathcal{C} is the phase velocity.

The generalized 3×3 Christoffel matrix in solid media is symmetric ($\Gamma_{ik} = \Gamma_{ki}$), positive definite ($\Gamma_{ik}a_i a_k > 0$, where a_i are components of any non-vanishing real-valued vector) and homogeneous function of the second degree in p_i ($\Gamma_{ik}(x_n, ap_j) = a^2 \Gamma_{ik}(x_n, p_j)$ for any non-vanishing constant a). It has three real-valued positive eigenvalues $G_m(x_n, p_j)$, and three corresponding real-valued unit eigenvectors $\mathbf{g}^{(m)}(x_n, p_j)$, $m = 1, 2, 3$. G_m and $\mathbf{g}^{(m)}$ are solutions of the eigenvalue equation

$$(\Gamma_{ik} - \delta_{ik}G_m)g_k^{(m)} = 0 , \quad i = 1, 2, 3 . \quad (9)$$

Eigenvectors $\mathbf{g}^{(1)}$, $\mathbf{g}^{(2)}$, $\mathbf{g}^{(3)}$ are mutually perpendicular. Eigenvalue G_m and the relevant eigenvector $\mathbf{g}^{(m)}$ are mutually related as follows:

$$G_m = \Gamma_{ik} g_i^{(m)} g_k^{(m)} = a_{ijkl} p_j p_l g_i^{(m)} g_k^{(m)} . \quad (10)$$

For transformation from anisotropic to isotropic media, it is sufficient to specify elastic moduli $c_{ijkl}(x_n)$ in terms of Lamé's elastic moduli $\lambda(x_n)$ and $\mu(x_n)$, describing isotropic media, as follows:

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) . \quad (11)$$

The element of the generalized Christoffel matrix is then given by the relation:

$$\Gamma_{ik} = \frac{\lambda + \mu}{\rho} p_i p_k + \frac{\mu}{\rho} \delta_{ik} p_n p_n . \quad (12)$$

In isotropic media, the expressions for eigenvalues and eigenvectors of the generalized Christoffel matrix can be determined analytically:

$$G_1 = G_2 = \beta^2 p_k p_k , \quad G_3 = \alpha^2 p_k p_k . \quad (13)$$

Here

$$\alpha^2 = (\lambda + 2\mu)/\rho , \quad \beta^2 = \mu/\rho . \quad (14)$$

The eigenvector relevant to the eigenvalue G_3 equals \mathbf{n} , the unit vector perpendicular to the wavefront. The eigenvectors relevant to coinciding eigenvalues G_1 and G_2 are mutually perpendicular unit vectors situated arbitrarily in the plane perpendicular to \mathbf{n} .

Eikonal equation. Polarization vector

The comparison of the basic equation of the ray method (6) with the eigenvalue equation (9) for the 3×3 generalized Christoffel matrix shows that equation (6) is satisfied, if the eigenvalue G_m of the generalized Christoffel matrix satisfies the relation

$$G_m(x_i, p_j) = 1 , \quad (15)$$

and if the complex-valued vectorial amplitude \mathbf{U} of the wave under consideration is related to eigenvector $\mathbf{g}^{(m)}$ as follows:

$$\mathbf{U} = A \mathbf{g}^{(m)} . \quad (16)$$

Equation (15) is the important *eikonal equation*. It is a nonlinear, first-order partial differential equation for travel time $T(x_n)$. Equation (16) shows that displacement vector \mathbf{U} is parallel to the appropriate eigenvector $\mathbf{g}^{(m)}$. For this reason, we call $\mathbf{g}^{(m)}$ the *polarization vector*. Symbol $A(x_n)$ denotes the complex-valued, frequency-independent, *scalar amplitude*.

Taking into account that G_m is a homogeneous function of the second degree in p_i , where $\mathbf{p} = \mathcal{C}^{-1} \mathbf{n}$, we obtain $G_m(x_i, p_j) = \mathcal{C}^{-2} G_m(x_i, n_j)$. This, (15) and (10) yield

$$\mathcal{C}^2(x_i, n_j) = G_m(x_i, n_j) = a_{ijkl} n_j n_l g_i^{(m)} g_k^{(m)} . \quad (17)$$

Phase velocity \mathcal{C} is the velocity of the wavefront in direction \mathbf{n} . The phase-velocity vector $\mathbf{C} = \mathcal{C}(x_i, n_j)\mathbf{n}$ has the direction of \mathbf{n} , i.e. it is perpendicular to the wavefront. It follows from (17) that the squares of phase velocity \mathcal{C} are eigenvalues $G_m(x_i, n_j)$ of the classical Christoffel matrix with elements $a_{ijkl}n_jn_l$.

Generally, eigenvalues G_m , $m = 1, 2, 3$, of the generalized Christoffel matrix are mutually different. They correspond to three high-frequency body waves propagating in inhomogeneous anisotropic media. We assign G_1 and G_2 to S1 and S2 waves and G_3 to P wave. If the eigenvalues are different, their polarization vectors can be determined uniquely.

If two eigenvalues coincide, we speak of the *degenerate case*. The corresponding eigenvectors can then be chosen as mutually perpendicular vectors situated arbitrarily in the plane perpendicular to the third eigenvector. Eigenvalues G_m may coincide *locally*, along certain lines or at certain points, which correspond to the so-called *S-wave singular directions*, or may be close to one another *globally* in a vicinity of singular directions or in *weakly anisotropic media*. The approximate but unique determination of polarization vectors in the latter situations is possible using perturbation approach (Jech and Pšenčík, 1989).

In isotropic media, the S-wave eigenvalues G_1 and G_2 coincide *globally*, see (13). Consequently, in isotropic media, the S waves are controlled by a single eikonal equation and we have thus only two different eikonal equations corresponding to P and S waves. As the equations for the eigenvalues in isotropic media can be determined analytically, we can express the eikonal equations for P and S waves explicitly:

$$\alpha^2 p_k p_k = 1 \quad \text{for P waves ,} \quad (18)$$

$$\beta^2 p_k p_k = 1 \quad \text{for S waves .} \quad (19)$$

In isotropic media, the generally complex-valued amplitude vector \mathbf{U} can be expressed in the simple form (16) only for P waves. In this case the polarization vector $\mathbf{g}^{(3)} = \mathbf{n}$, i.e. it is perpendicular to the wavefront. For S waves, \mathbf{U} must be considered in the following form:

$$\mathbf{U} = B\mathbf{g}^{(1)} + C\mathbf{g}^{(2)} . \quad (20)$$

Here $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ are two mutually perpendicular unit vectors in the plane tangent to the wavefront, i.e. perpendicular to the vector \mathbf{n} . The computation of $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ along the ray is explained later (see (37)). Symbols $B(x_n)$ and $C(x_n)$ are the corresponding, generally complex-valued scalar amplitudes.

In the seismic ray method, it is common to express the eikonal equation (15) in Hamiltonian form. Hamiltonian $\mathcal{H}(x_i, p_j)$ may be introduced in various ways. We shall consider the Hamiltonian, which is a homogeneous function of the second degree in p_i . For inhomogeneous anisotropic media, we can introduce the Hamiltonian expressed in terms of $G_m(x_i, p_j)$, see eq.(10):

$$\mathcal{H}(x_i, p_j) = \frac{1}{2}G_m(x_i, p_j) = \frac{1}{2}a_{ijkl}n_jn_lg_i^{(m)}g_k^{(m)} . \quad (21)$$

The eikonal equation (15) then reads:

$$\mathcal{H}(x_i, p_j) = \frac{1}{2} . \quad (22)$$

It holds for anisotropic as well as isotropic media.

From (13) and (21), we get for isotropic inhomogeneous media:

$$\mathcal{H}(x_i, p_j) = \frac{1}{2} V^2(x_i) p_k p_k , \quad (23)$$

where $V = \alpha$ for P waves and $V = \beta$ for S waves.

Ray tracing and travel-time computation

The eikonal equation in Hamiltonian form (22), with $p_j = \partial T / \partial x_j$, is a non-linear partial differential equation of the first order for travel time $T(x_i)$. It can be solved by the method of characteristics. The characteristics of eikonal equation (22) are spatial trajectories, along which (22) is satisfied, and along which travel time T can be computed by quadratures. The characteristics of the eikonal equation represent *rays*.

The characteristics of the eikonal equation expressed in general Hamiltonian form are described by a system of generally non-linear, ordinary differential equations of the first order:

$$\frac{dx_i}{du} = \frac{\partial \mathcal{H}}{\partial p_i} , \quad \frac{dp_i}{du} = - \frac{\partial \mathcal{H}}{\partial x_i} , \quad \frac{dT}{du} = p_k \frac{\partial \mathcal{H}}{\partial p_k} . \quad (24)$$

Here u is a real-valued parameter along the ray. The relation between parameter u and the travel time along the ray depends on the form of the Hamiltonian used, see the last equation in (24). For Hamiltonians, which are homogeneous functions of the second degree in p_i , the Euler equation for homogeneous functions yields $p_k \partial \mathcal{H} / \partial p_k = 2\mathcal{H}$. If we consider Hamiltonian (21), we get $dT/du = 1$ from (24). For travel time T along the ray, denoted $\tau = T$, eqs (24) simplify to:

$$\frac{dx_i}{d\tau} = \frac{\partial \mathcal{H}}{\partial p_i} , \quad \frac{dp_i}{d\tau} = - \frac{\partial \mathcal{H}}{\partial x_i} . \quad (25)$$

This system of equations is usually called the *ray tracing system*. Solution of the ray tracing system (25) with appropriate initial conditions yields $x_i(\tau)$, the coordinates of points along the ray trajectory, and $p_i(\tau)$, the Cartesian components of the slowness vectors along the ray. The travel time T along the ray is obtained automatically, $T = \tau$.

Inserting (21) in (25), we obtain the ray tracing system for m -th wave in inhomogeneous anisotropic media:

$$\frac{dx_i}{d\tau} = a_{ijkl} p_l g_j^{(m)} g_k^{(m)} , \quad \frac{dp_i}{d\tau} = - \frac{1}{2} \frac{\partial a_{jklm}}{\partial x_i} p_k p_n g_j^{(m)} g_l^{(m)} . \quad (26)$$

In the derivation of the first equation of (26) for $\partial \mathcal{H} / \partial p_i$, we took into account that $\Gamma_{ik} \partial (g_i^{(m)} g_k^{(m)}) / \partial p_n = 0$. Ray-tracing equations (26) represent an alternative version of ray-tracing equations derived by Červený (1972).

The initial conditions for the ray tracing system (26) are $x_i = x_{0i}$, $p_i = p_{0i}$, where x_{0i} and p_{0i} satisfy the eikonal equation (22), corresponding to the wave we wish to compute (P, S1 or S2). Components p_{0i} of the initial slowness vector \mathbf{p}_0 can be then expressed as $p_{0i} = n_{0i}/\mathcal{C}(x_{0i})$, where \mathcal{C} is the relevant phase velocity. The eikonal equation (22) is then satisfied along the whole ray.

In inhomogeneous isotropic media, the ray tracing system (26) reduces to

$$\frac{dx_i}{d\tau} = V^2 p_i, \quad \frac{dp_i}{d\tau} = -\frac{\partial \ln V}{\partial x_i}. \quad (27)$$

The initial conditions for the ray tracing system (27) are again $x_i = x_{0i}$, $p_i = p_{0i}$, where $p_{0i} = n_{0i}/V(x_{0i})$. Here $V = \alpha$ for P waves, and $V = \beta$ for S waves.

As τ is the travel time along the ray, $dx_i/d\tau$ represent the Cartesian components \mathcal{U}_i of the *ray-velocity vector* \mathcal{U} of the m -th wave:

$$\mathcal{U}_i = a_{ijkl} p_l g_j^{(m)} g_k^{(m)}. \quad (28)$$

In non-dissipative anisotropic media, the ray-velocity vector \mathcal{U} is also called the group velocity vector or the energy velocity vector.

In anisotropic media, the ray-velocity vector \mathcal{U} must be strictly distinguished from the phase velocity vector \mathcal{C} . In inhomogeneous anisotropic media, the ray-velocity and phase-velocity vectors \mathcal{U} and \mathcal{C} are generally different, both in size and direction. Vector \mathcal{U} is always greater than \mathcal{C} . The two vectors are equal (in size and direction) only in special directions, called *longitudinal directions*.

In inhomogeneous isotropic media, eq.(28) for the ray-velocity vector yields $\mathcal{U} = V^2 \mathbf{p}$. For the phase-velocity vector, using (17), we get $\mathcal{C} = V^2 \mathbf{p}$. In both cases, $V = \alpha$ for P waves, and $V = \beta$ for S waves. Thus, the ray-velocity and phase-velocity vectors are identical in isotropic media.

Ray tracing systems (26) and (27) can be simply solved if the initial values x_{0i} and p_{0i} are specified at some point S of the ray. We then speak of *initial-value ray tracing*. The standard numerical procedures of solving the system of ordinary differential equations of the first order with specified initial conditions can then be used (Runge-Kutta, etc.). A very important role in seismology is played by *boundary-value ray tracing*, in which we seek the ray, satisfying some boundary conditions. The typical boundary value problem is *two-point ray tracing*, in which we seek the ray connecting two specified points. Mostly, the controlled initial-value ray tracing (controlled shooting method) is used to solve this problem (Červený et al., 2007). Boundary value ray tracing is considerably more complicated than initial-value ray tracing.

There are four important differences between initial value ray tracing in isotropic and anisotropic media. First: In anisotropic media, we deal with three waves, P, S1 and S2, in isotropic media with two waves, P and S, only. Second: In inhomogeneous anisotropic media, ray-tracing system (26) is the same for all three waves. The wave under consideration is specified by the initial conditions, which must satisfy the eikonal equation of the considered wave. In isotropic inhomogeneous media, the ray tracing systems are

explicit for P and S waves, see (27) with $V = \alpha$ and $V = \beta$, respectively. Third: In isotropic media, the initial direction of the slowness vector specifies directly the initial direction of the ray (as the tangent to the ray and the slowness vector have the same directions). In anisotropic media, the direction of the ray is, generally, different from the direction of the slowness vector. Nevertheless, we can use p_{0i} as the initial values for the ray tracing system. The ray-velocity vector \mathbf{u} can be simply calculated from slowness vector \mathbf{p} at any point of the ray, including the initial point. Fourth: Ray tracing for P and S waves is regular everywhere in inhomogeneous isotropic media. In anisotropic media, problems arise with tracing S-wave rays in vicinities of singular directions, or if anisotropy is weak.

The problem of ray tracing and travel-time computation in inhomogeneous media has been broadly discussed in the seismological literature; particularly for inhomogeneous isotropic media. Many ray tracing systems and many suitable numerical procedures for performing ray tracing have been proposed. For 1-D isotropic media (vertically inhomogeneous, radially symmetric), the ray tracing systems may be simplified so that they reduce to simple quadratures, well-known from classical seismological textbooks (Aki and Richards, 1980). Standard programs for ray tracing and travel-time computations in laterally varying isotropic and anisotropic structures are available, see, for example, program packages SEIS (2D isotropic models), CRT and ANRAY (3D isotropic/anisotropic models) at <http://sw3d.cz/>. Programs for anisotropic media have, however, problems with S-wave computations when anisotropy is weak and in the vicinities of shear-wave singularities. In such cases, the standard ray theory should be replaced by the coupling ray theory. Numerical procedures based on the coupling ray theory are, unfortunately, rare.

Ray tracing may also serve as a basis for the so-called *wavefront construction method* (Gjøystdal et al., 2002). In this case, for a selected wave, wavefronts with travel times $T = T_0 + k\Delta T$ are computed successively from the previous wavefronts with travel times $T = T_0 + (k - 1)\Delta T$. The wavefront construction method has found broad applications in seismic exploration.

Let us consider a two-parametric system of rays, call it the *ray field*, and specify the individual rays in the ray field by *ray parameters* γ_1, γ_2 . Ray parameters γ_1, γ_2 may represent, e.g., the take-off angles at a point source, or the curvilinear Gaussian coordinates of initial ray points along the initial surface. The family of rays with ray parameters within the limit $[\gamma_1, \gamma_1 + d\gamma_1], [\gamma_2, \gamma_2 + d\gamma_2]$, is called the *ray tube*. We further introduce *ray coordinates* $\gamma_1, \gamma_2, \gamma_3$ in such a way that γ_1, γ_2 are ray parameters, and γ_3 is some monotonic parameter along a ray (arclength s , travel time τ , etc.). Here we consider $\gamma_3 = \tau$, but our results may be simply modified for any other monotonic parameter γ_3 . We further introduce the 3×3 transformation matrix $\hat{\mathbf{Q}}$ from ray to Cartesian coordinates with elements $Q_{ij} = \partial x_i / \partial \gamma_j$. The Jacobian of transformation from ray to Cartesian coordinates, $\det \hat{\mathbf{Q}}$, can be expressed as follows:

$$\det \hat{\mathbf{Q}}(\tau) = (\partial \mathbf{x}(\tau) / \partial \gamma_1 \times \partial \mathbf{x}(\tau) / \partial \gamma_2)^T \mathbf{u}(\tau) . \quad (29)$$

The vectorial product in (29) has the direction of the normal to the wavefront, specified by $\mathbf{n} = \mathcal{C}\mathbf{p}$. As $\mathbf{p}(\tau) \cdot \mathbf{u}(\tau) = 1$, see (28), (10) and (15), we also obtain

$$\det \hat{\mathbf{Q}}(\tau) = \pm \mathcal{C}(\tau) |(\partial \mathbf{x}(\tau) / \partial \gamma_1 \times \partial \mathbf{x}(\tau) / \partial \gamma_2)| . \quad (30)$$

Thus, Jacobian $\det \hat{\mathbf{Q}}(\tau)$ measures the cross-sectional area of the ray tube, i.e. it measures the density of rays, and the expansion or contraction of the ray tube. For this reason, the 3×3 matrix $\hat{\mathbf{Q}}(\tau)$ is also often called the *geometrical spreading matrix* and $J(\tau) = (\mathcal{U}^{-1}(\tau) \det \hat{\mathbf{Q}}(\tau))^{1/2}$ *geometrical spreading*. It plays an important role in the computation of the ray-theory amplitudes.

Transport equation. Computation of ray-theory amplitudes

The second equation of the basic system of equations of the ray method yields the transport equation for the scalar ray-theory amplitude $A(x_i)$. The transport equation is a partial differential equation of the first order. It can be expressed in several forms. One of them reads

$$\nabla \cdot (\rho A^2 \mathbf{u}) = 0 . \quad (31)$$

It is common to solve the transport equation along the ray. $\nabla \cdot \mathbf{u}$ can then be expressed as follows:

$$\nabla \cdot \mathbf{u} = d[\ln(\det \hat{\mathbf{Q}})]/d\tau \quad (32)$$

(Červený, 2001, eq.(3.10.24)). Inserting (32) into (31) yields the transport equation in the form of the first-order ordinary differential equation along the ray:

$$d \left(\rho(\tau) A^2(\tau) \det \hat{\mathbf{Q}}(\tau) \right) / d\tau = 0 . \quad (33)$$

This yields a simple form of the continuation relation for $A(\tau)$ along the ray:

$$A(\tau) = \left[\frac{\rho(\tau_0) \det \hat{\mathbf{Q}}(\tau_0)}{\rho(\tau) \det \hat{\mathbf{Q}}(\tau)} \right]^{1/2} A(\tau_0) . \quad (34)$$

We obtain another suitable continuation relation for amplitudes along the ray by introducing a special local Cartesian coordinate system y_1, y_2, y_3 , varying along the ray. We call it the *wavefront orthonormal coordinate system*. At any point of the ray specified by $\gamma_3 = \tau$, the y_3 axis is parallel to slowness vector \mathbf{p} , and the y_1, y_2 axes are confined to the plane tangential to the wavefront at $\gamma_3 = \tau$. Axes y_1 and y_2 are mutually perpendicular. If we denote the 3×3 transformation matrix from ray coordinates to wavefront orthonormal coordinates by $\hat{\mathbf{Q}}^{(y)}$, then

$$\det \hat{\mathbf{Q}}(\tau) = \det \hat{\mathbf{Q}}^{(y)}(\tau) = \mathcal{C}(\tau) \det \mathbf{Q}^{(y)}(\tau) . \quad (35)$$

Here $\mathcal{C}(\tau)$ is the phase velocity, and $\mathbf{Q}^{(y)}(\tau)$ is the 2×2 upper-left submatrix of $\hat{\mathbf{Q}}^{(y)}(\tau)$. Using (35) in (34), we obtain the continuation relation in an alternative form:

$$A(\tau) = \left[\frac{\rho(\tau_0) \mathcal{C}(\tau_0) \det \mathbf{Q}^{(y)}(\tau_0)}{\rho(\tau) \mathcal{C}(\tau) \det \mathbf{Q}^{(y)}(\tau)} \right]^{1/2} A(\tau_0) . \quad (36)$$

An important property of continuation relation (36) is that $\det \mathbf{Q}^{(y)}(\tau)$ is uniquely determined by coordinates y_1 and y_2 , confined to the plane tangential to the wavefront at τ .

Thus, (36) remains valid for any coordinate systems q_i (even nonorthogonal), in which the coordinate axes q_1 and q_2 are confined to the plane tangential to the wavefront, but the axis q_3 is taken in a different way than y_3 , for example along the ray. This is, e.g., the case of the well-known *ray-centred coordinate system* q_1, q_2, q_3 , in which $\det \mathbf{Q}^{(y)}(\tau) = \det \mathbf{Q}^{(q)}(\tau)$.

Transport equations for P and S waves in isotropic media may be also transformed into the form (31). The transformation is straightforward for P waves. Transport equations for scalar amplitudes B and C in (20) are generally coupled. They decouple only if the unit vectors $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ in (20) satisfy the following relation along the ray:

$$d\mathbf{g}^{(M)}/d\tau = (\mathbf{g}^{(M)} \cdot \nabla\beta)\mathbf{n}, \quad M = 1, 2. \quad (37)$$

In the terminology of the Riemannian geometry, vector $\mathbf{g}^{(M)}$ satisfying (37) is transported parallelly along the ray. If $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ are chosen as mutually perpendicular and perpendicular to \mathbf{n} at one point of the ray, equation (37) guarantees that they have these properties at any point of the ray. Consequently, $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ are always perpendicular to the ray and do not rotate around it as the S wave progresses. As $\mathbf{g}^{(1)}$, $\mathbf{g}^{(2)}$ and \mathbf{n} are always orthonormal, and \mathbf{n} is known at any point of the ray, it is not necessary to use (37) to compute both vectors $\mathbf{g}^{(M)}$. One of them can be determined from the orthonormality condition.

Quantity $\det \hat{\mathbf{Q}}(\tau)$ in eq.(34) may be zero at some point $\tau = \tau^C$. This means that the cross-sectional area of the ray tube shrinks to zero at $\tau = \tau^C$. The relevant point $\tau = \tau^C$ of the ray is called the *caustic point*. At the caustic point, the ray solution is singular and yields an infinite amplitude there. In passing through the caustic point τ^C along the ray, the argument of $[\det \hat{\mathbf{Q}}(\tau)]^{1/2}$ may change by $\pm\pi/2$ or $\pm\pi$ (Kravtsov and Orlov, 1999). It is common to introduce the **phase shift due to caustic** $T^C(\tau, \tau_0)$ using the relation

$$\left[\frac{\det \hat{\mathbf{Q}}(\tau_0)}{\det \hat{\mathbf{Q}}(\tau)} \right]^{1/2} = \left| \frac{\det \hat{\mathbf{Q}}(\tau_0)}{\det \hat{\mathbf{Q}}(\tau)} \right|^{1/2} \exp[iT^C(\tau, \tau_0)] \quad (38)$$

if caustic point τ^C is situated between τ_0 and τ . The phase shift due to the caustic is cumulative. If the ray passes through several caustic points along the ray between τ_0 and τ , the phase shift due to caustics is the sum of the individual phase shifts. It is often expressed in the form $T^C(\tau, \tau_0) = -\frac{1}{2}\pi k(\tau, \tau_0)$, where $k(\tau, \tau_0)$ is an integer, called the KMAH index (to acknowledge the work by Keller, Maslov, Arnold and Hörmander in this field). The continuation relation for ray-theory amplitudes (34) can then be modified to read:

$$A(\tau) = \left(\frac{\rho(\tau_0) |\det \hat{\mathbf{Q}}(\tau_0)|}{\rho(\tau) |\det \hat{\mathbf{Q}}(\tau)|} \right)^{1/2} \exp[iT^C(\tau, \tau_0)] A(\tau_0). \quad (39)$$

Equation (36) can be transformed to the analogous form as (39) as the zeros of $\det \mathbf{Q}^{(y)}(\tau)$ are situated at the same points τ^C on the ray as the zeros of $\det \hat{\mathbf{Q}}(\tau)$.

The KMAH index can be calculated along the ray as a byproduct of dynamic ray tracing. For detailed derivations and discussion see Bakker (1998) and Klimeš (2010).

There are some differences between the KMAH indices along the rays in isotropic and anisotropic media. In isotropic media, the KMAH index always increases when the ray

passes through a new caustic point, either by one or two. In anisotropic media, however, it may also decrease by one or two at some caustic points. This happens only for S waves as a consequence of the concave form of the slowness surface of the corresponding S wave.

Dynamic ray tracing. Paraxial approximations

As we can see in (34), the computation of the ray-theory amplitudes requires knowledge of $\det \hat{\mathbf{Q}}$, where $\hat{\mathbf{Q}}(\tau)$ characterizes the properties of the ray field in the vicinity of the ray under consideration. $\hat{\mathbf{Q}}(\tau)$ can be computed by the procedure called *dynamic* (or paraxial) *ray tracing*. In addition to $\hat{\mathbf{Q}}(\tau)$ with elements $Q_{ij}(\tau)$, we also have to introduce a new 3×3 matrix $\hat{\mathbf{P}}(\tau)$ with elements $P_{ij}(\tau) = \partial p_i / \partial \gamma_j$. The equation for P_{ij} must be included to obtain the linear dynamic ray tracing system. Differentiating ray tracing system (25) with respect to γ_j , we can easily obtain a system of linear ordinary differential equations of the first order in Q_{ij} and P_{ij} ,

$$\begin{aligned} \frac{dQ_{ij}}{d\tau} &= \frac{\partial^2 \mathcal{H}}{\partial p_i \partial x_k} Q_{kj} + \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_k} P_{kj} , \\ \frac{dP_{ij}}{d\tau} &= -\frac{\partial^2 \mathcal{H}}{\partial x_i \partial x_k} Q_{kj} - \frac{\partial^2 \mathcal{H}}{\partial x_i \partial p_k} P_{kj} . \end{aligned} \quad (40)$$

This system is usually called the *dynamic ray tracing system*, and the relevant procedure dynamic ray tracing (Červený, 1972). It can be solved along a given ray, or together with it.

The dynamic ray tracing system (40) may be expressed in various forms. Instead of Cartesian coordinates x_i , we can use the wavefront orthonormal coordinates y_i , or the ray-centred coordinates q_i . Then, instead of the 3×3 matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{P}}$, it is sufficient to seek the 2×2 matrices $\mathbf{Q}^{(y)}$, $\mathbf{P}^{(y)}$ or $\mathbf{Q}^{(q)}$, $\mathbf{P}^{(q)}$. This reduces the number of DRT equations, but complicates their right-hand sides (Červený 2001; Sec. 4.2).

As the dynamic ray tracing system (40) is of the first order and linear, we can compute its fundamental matrix consisting of six linearly independent solutions. The 6×6 fundamental matrix of (40) specified by the 6×6 identity matrix at an arbitrary point $\tau = \tau_0$ of the ray is called the *ray propagator matrix* and denoted by $\mathbf{\Pi}(\tau, \tau_0)$.

The 6×6 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ is symplectic:

$$\mathbf{\Pi}^T(\tau, \tau_0) \mathbf{J} \mathbf{\Pi}(\tau, \tau_0) = \mathbf{J} , \quad \text{with} \quad \mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix} . \quad (41)$$

If we know the matrices $\hat{\mathbf{Q}}(\tau_0)$, $\hat{\mathbf{P}}(\tau_0)$, we can compute $\hat{\mathbf{Q}}(\tau)$, $\hat{\mathbf{P}}(\tau)$ at any point τ of the ray by simple matrix multiplication

$$\begin{pmatrix} \hat{\mathbf{Q}}(\tau) \\ \hat{\mathbf{P}}(\tau) \end{pmatrix} = \mathbf{\Pi}(\tau, \tau_0) \begin{pmatrix} \hat{\mathbf{Q}}(\tau_0) \\ \hat{\mathbf{P}}(\tau_0) \end{pmatrix} . \quad (42)$$

The ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ satisfies the chain rule, $\mathbf{\Pi}(\tau, \tau_0) = \mathbf{\Pi}(\tau, \tau_1) \mathbf{\Pi}(\tau_1, \tau_0)$, where point τ_1 is situated arbitrarily on the ray. It is simple to compute the inverse of

$\mathbf{\Pi}(\tau, \tau_0)$: $\mathbf{\Pi}^{-1}(\tau, \tau_0) = \mathbf{\Pi}(\tau_0, \tau)$. We can express $\mathbf{\Pi}(\tau, \tau_0)$ in the following way:

$$\mathbf{\Pi}(\tau, \tau_0) = \begin{pmatrix} \hat{\mathbf{Q}}_1(\tau, \tau_0) & \hat{\mathbf{Q}}_2(\tau, \tau_0) \\ \hat{\mathbf{P}}_1(\tau, \tau_0) & \hat{\mathbf{P}}_2(\tau, \tau_0) \end{pmatrix}, \quad (43)$$

where $\hat{\mathbf{Q}}_1(\tau, \tau_0)$, $\hat{\mathbf{Q}}_2(\tau, \tau_0)$, $\hat{\mathbf{P}}_1(\tau, \tau_0)$ and $\hat{\mathbf{P}}_2(\tau, \tau_0)$ are 3×3 matrices.

Eq.(42) can be used to obtain a very important quantity - the 3×3 matrix $\hat{\mathbf{M}}(\tau)$ of second derivatives of the travel-time field with respect to Cartesian coordinates, with elements $M_{ij} = \partial^2 T / \partial x_i \partial x_j$:

$$\hat{\mathbf{M}}(\tau) = \hat{\mathbf{P}}(\tau)(\hat{\mathbf{Q}}(\tau))^{-1}. \quad (44)$$

Matrix $\hat{\mathbf{M}}(\tau)$ plays an important role in the computation of travel time not only along the ray, but also in its "quadratic" paraxial vicinity:

$$T(\mathbf{x}) = T(\mathbf{x}^\Omega) + (\mathbf{x} - \mathbf{x}^\Omega)^T \mathbf{p}(\tau) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^\Omega)^T \hat{\mathbf{M}}(\tau)(\mathbf{x} - \mathbf{x}^\Omega). \quad (45)$$

In (45), \mathbf{x} denotes an arbitrary point in the paraxial vicinity of the ray, close to point $\mathbf{x}^\Omega = \mathbf{x}^\Omega(\tau)$ on the ray, slowness vector $\mathbf{p}(\tau)$ and the matrix $\hat{\mathbf{M}}(\tau)$ are given at \mathbf{x}^Ω . The possibility of computing the travel time in the paraxial vicinity of the ray has many important applications.

The properties of the 6×6 ray propagator matrix $\mathbf{\Pi}(\tau, \tau_0)$ described above remain valid even for the 4×4 ray propagator matrices $\mathbf{\Pi}^{(y)}(\tau, \tau_0)$ or $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ expressed in wavefront orthonormal coordinates y_i or ray-centred coordinates q_i . The ray propagator matrices $\mathbf{\Pi}^{(y)}(\tau, \tau_0)$ and $\mathbf{\Pi}^{(q)}(\tau, \tau_0)$ are identical, therefore, the 2×2 matrices $\mathbf{Q}_1(\tau, \tau_0)$, $\mathbf{Q}_2(\tau, \tau_0)$, $\mathbf{P}_1(\tau, \tau_0)$ and $\mathbf{P}_2(\tau, \tau_0)$ are the same. Matrices $\mathbf{Q}_1(\tau, \tau_0)$, $\mathbf{P}_1(\tau, \tau_0)$ correspond to the plane-wavefront initial conditions at τ_0 , and matrices $\mathbf{Q}_2(\tau, \tau_0)$, $\mathbf{P}_2(\tau, \tau_0)$ to the point-source initial conditions at τ_0 . The 2×2 matrix $\mathbf{Q}_2(\tau, \tau_0)$ plays an important role in computing the ray-theory Green function. The quantity

$$\mathcal{L}(\tau, \tau_0) = |\det \mathbf{Q}_2(\tau, \tau_0)|^{1/2} \quad (46)$$

is called the *relative geometrical spreading*. It corresponds to a point source.

As in (44), we can define the 2×2 matrix of the second derivatives of the travel-time field with respect to y_1, y_2 or q_1, q_2 as follows:

$$\mathbf{M}(\tau) = \mathbf{P}(\tau)(\mathbf{Q}(\tau))^{-1}. \quad (47)$$

We will now briefly summarize several useful ray-theory quantities and applications, which rely fully or partly on dynamic ray tracing. For derivations and more detailed explanations, see Červený (2001, Chap.4), where also many other applications and references can be found: 1) Paraxial travel times. 2) Paraxial slowness vectors. 3) Paraxial rays. 4) Curvature of the wavefront. 5) Matrix of geometrical spreading $\hat{\mathbf{Q}}$ and the relevant matrix $\hat{\mathbf{P}}$. 6) Continuation relations for ray-theory amplitudes along the ray. 7) Relative geometrical spreading. 8) Phase shift due to caustics. 9) Ray-theory elastodynamic Green

function. 10) Higher-order spatial derivatives of the travel-time field. 11) Fresnel volumes and Fresnel zones. 12) Surface-to-surface propagator matrix. 13) Boundary-value problems in four parametric system of paraxial rays, including two-point ray tracing. 14) Factorization of the geometrical spreading.

Dynamic ray tracing is also needed in the investigation of ray chaos and in computations of Lyapunov exponents, in the ray-perturbation methods and in modifications and extensions of the ray method such as Maslov method, Gaussian beam and Gaussian packet summation methods, in Kirchhoff-Helmholtz method and in various diffraction methods.

Coupling ray theory for S waves

In inhomogeneous weakly anisotropic media, the standard ray theory described above, yields distorted results since it is unable to describe the coupling of S1 and S2 waves propagating with approximately equal phase velocities. This problem can be removed by using the coupling ray theory. In the coupling ray theory, the amplitudes of the two S waves can be computed along a trajectory called the *common ray* (Bakker, 2002; Klimeš, 2006). The closer the common ray approximates actual S-wave rays, the more accurate results the coupling ray theory yields. The common rays can be constructed in a reference isotropic medium or in the actual anisotropic medium. A convenient option is to compute common rays using ray-tracing equations (25) with Hamiltonian given as

$$\mathcal{H}(x_i, p_j) = \frac{1}{4}[G_1(x_i, p_j) + G_2(x_i, p_j)] . \quad (48)$$

In (48), G_1 and G_2 are eigenvalues of the Christoffel matrix (7), corresponding to S1 and S2 waves.

The coupling ray theory solution is sought in the form (Coates and Chapman, 1990; Bulant and Klimeš, 2002):

$$\mathbf{u}(\tau, t) = A(\tau)[r_1(\tau)\mathbf{g}^{(1)}(\tau) \exp(i\omega\tau_1) + r_2(\tau)\mathbf{g}^{(2)}(\tau) \exp(i\omega\tau_2)] \exp(-i\omega t) . \quad (49)$$

Here, $A(\tau)$ is the scalar amplitude (34) or (36) calculated along the common ray. The symbols $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ denote the eigenvectors of the Christoffel matrix $\mathbf{\Gamma}$ calculated along the common ray. The eigenvectors $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ correspond to S waves. The travel times τ_1 and τ_2 are travel times corresponding to the above vectors $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$. They can be obtained by quadratures along the common ray:

$$d\tau_1/d\tau = [\Gamma_{ik}g_i^{(1)}g_k^{(1)}]^{-1/2} , \quad d\tau_2/d\tau = [\Gamma_{ik}g_i^{(2)}g_k^{(2)}]^{-1/2} . \quad (50)$$

The amplitude factors r_1 and r_2 are solutions of two coupled ordinary differential equations (Coates and Chapman, 1990):

$$\begin{pmatrix} dr_1/d\tau \\ dr_2/d\tau \end{pmatrix} = \frac{d\varphi}{d\tau} \begin{pmatrix} 0 & \exp(i\omega[\tau_2(\tau) - \tau_1(\tau)]) \\ -\exp(i\omega[\tau_1(\tau) - \tau_2(\tau)]) & 0 \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \end{pmatrix} , \quad (51)$$

where the angular velocity $d\varphi/d\tau$ of the rotation of the eigenvectors $\mathbf{g}^{(1)}$ and $\mathbf{g}^{(2)}$ is given by

$$\frac{d\varphi}{d\tau} = \mathbf{g}^{(2)} \frac{d\mathbf{g}^{(1)}}{d\tau} = -\mathbf{g}^{(1)} \frac{d\mathbf{g}^{(2)}}{d\tau} . \quad (52)$$

For detailed description of the algorithm, see Bulant and Klimeš (2002).

There are many possible modifications and approximations of the coupling ray theory. In some of them, the amplitude vector \mathbf{U} of coupled S waves is sought along the common ray in the form (20), in which the amplitude factors B and C can be expressed as

$$B(\tau) = A(\tau)\mathcal{B}(\tau) \quad C(\tau) = A(\tau)\mathcal{C}(\tau) . \quad (53)$$

In (53), $A(\tau)$ is again the scalar ray amplitude (34) or (36) calculated along the common S-wave ray. There are many ways how to evaluate factors \mathcal{B} and \mathcal{C} (Kravtsov, 1968; Pšenčík, 1998; Červený et al., 2007). Here we present a combination of coupling ray theory and of the first-order ray tracing (Farra and Pšenčík, 2010, see also section on ray perturbation methods). In the approximation of Farra and Pšenčík (2010), the common ray is obtained as the first-order ray. The vectors $\mathbf{g}^{(K)}$, appearing in (20), specify the first-order approximation of the S-wave polarization plane. The factors \mathcal{B} and \mathcal{C} in (53) are then obtained as a solution of two coupled ordinary differential equations, which result from the corresponding transport equations:

$$\begin{pmatrix} d\mathcal{B}/d\tau \\ d\mathcal{C}/d\tau \end{pmatrix} = -\frac{i\omega}{2} \begin{pmatrix} \mathcal{M}_{11} - 1 & \mathcal{M}_{12} \\ \mathcal{M}_{12} & \mathcal{M}_{22} - 1 \end{pmatrix} \begin{pmatrix} \mathcal{B} \\ \mathcal{C} \end{pmatrix} . \quad (54)$$

Evaluation of the matrix \mathcal{M} with elements \mathcal{M}_{IJ} is simple, see eqs (20) and (7) of Farra and Pšenčík (2010).

The resulting equations reduce to standard ray-theory equations in inhomogeneous isotropic media, they describe properly S-wave coupling in inhomogeneous weakly anisotropic media and even yield separate S waves when anisotropy is stronger. Common S-wave rays are regular everywhere. They do not suffer from problems well known from tracing rays of individual S waves in anisotropic media and are suitable for investigating shear-wave splitting.

Effects of structural interfaces

Assume that the ray is incident on a curved structural interface. If we wish to continue the ray computations for the reflected, transmitted, monotypic or converted waves, we have to use relevant transformation relations for the ray tracing system, dynamic ray tracing system and for the ray theory amplitudes.

The transformation relations for ray tracing and dynamic ray tracing systems at interfaces are well known (Červený, 2001). For the sake of brevity, we do not present them here. We shall, however, discuss the transformation of amplitudes. In the zero-order ray approximation, the transformation of ray-theory amplitudes across an interface is described by plane-wave reflection/transmission coefficients. Consequently, amplitudes of generated waves do not depend on the curvature of the wavefront of the incident wave and the curvature of the interface at the point of incidence Q . Neither do they depend on the gradients of the density and of the density-normalized elastic moduli at Q , on both sides of the interface. They depend only on the local values of the density and

density-normalized elastic moduli at Q (on both sides of the interface) and on the angle of incidence.

Various types of R/T coefficients may be used. The displacement R/T coefficients are used most frequently (Aki and Richards, 1980; Červený et al., 1977 for isotropic media; Fedorov, 1968 for anisotropic media). Very useful are the energy R/T coefficients, as they are reciprocal. The relation between the energy R/T coefficient $\mathcal{R}(Q)$ and the displacement R/T coefficient $R(Q)$ is as follows:

$$\mathcal{R}(Q) = R(Q) \left[\frac{\rho(\tilde{Q})\mathcal{U}_n(\tilde{Q})}{\rho(Q)\mathcal{U}_n(Q)} \right]^{1/2} \quad (55)$$

(Červený 2001; Sec.5.4.3). Here Q is the point of incidence, and \tilde{Q} the relevant initial point of the R/T wave, both points being, of course, identical. \mathcal{U}_n is the normal component (perpendicular to the interface) of the ray-velocity vector. We further introduce the complete energy R/T coefficients \mathcal{R}^C along the ray using the relation

$$\mathcal{R}^C = \prod_{k=1}^N \mathcal{R}(Q_k) . \quad (56)$$

The complete energy R/T coefficient \mathcal{R}^C corresponds to the ray which interacts N -times with interfaces (at points of incidence Q_1, Q_2, \dots, Q_N) between the initial and end point of the ray.

Generalization of the continuation relation (36) for the ray-theory amplitudes along the ray situated in a laterally varying anisotropic medium containing curved interfaces then reads:

$$A(\tau) = \left(\frac{\rho(\tau_0)\mathcal{C}(\tau_0) |\det \mathbf{Q}^{(y)}(\tau_0)|}{\rho(\tau)\mathcal{C}(\tau) |\det \mathbf{Q}^{(y)}(\tau)|} \right)^{1/2} \mathcal{R}^C \exp[iT^C(\tau, \tau_0)] A(\tau_0) . \quad (57)$$

In seismic prospecting, in the technique called *amplitude variation with offset* (AVO), it is common to work with the so-called *weak-contrast R/T coefficients*. They are linearized versions of exact R/T displacement coefficients. Linearization is mostly made with respect to the contrasts of the density and elastic moduli across the interface. There is a great variety of linearized formulae depending on the type of media surrounding the interface (isotropic, anisotropic), strength of anisotropy (weak, strong), etc. The coefficients yield reasonable approximation in the vicinity of normal incidence. For increasing incidence angles, their accuracy decreases. The advantage of the weak-contrast coefficients is their simplicity and the possibility of expressing them in explicit form. The effects of the individual medium parameters on the coefficients can then be easily evaluated.

Ray-theory elastodynamic Green function

The elastodynamic Green function $G_{in}(R, t, S, t_0)$ represents the i -th Cartesian component of the far-field displacement vector at location R and time t , due to a single-force

point source situated at location S and oriented along the n -th Cartesian axis, with the time dependence $\delta(t - t_0)$. We introduce quite analogously the ray-theory elastodynamic Green function, with only two differences. The first difference is that ray-theory Green function is defined as a sum of *elementary ray-theory Green functions* computed along rays of selected elementary waves (direct, multiply reflected/transmitted, etc.). The second difference is that the elementary ray-theory Green functions are not exact, but only zero-order ray approximations.

The Fourier transform $G_{in}(R, S, \omega)$ of the elementary ray-theory elastodynamic Green function $G_{in}(R, t, S, t_0)$ with respect to $t - t_0$ then reads

$$G_{in}(R, S, \omega) = \frac{g_n(S)g_i(R) \exp[iT^G(R, S) - i\omega\tau(R, S)]}{4\pi[\rho(S)\rho(R)\mathcal{C}(S)\mathcal{C}(R)]^{1/2}\mathcal{L}(R, S)} \mathcal{R}^C . \quad (58)$$

Here $\mathcal{L}(R, S)$ is the relative geometrical spreading, given by (46), $g_i(R)$ and $g_n(S)$ are the eigenvectors of the generalized Christoffel matrix at R and S (polarization vectors corresponding to the considered elementary wave), $\tau(R, S)$ is the travel time along the ray from S to R , \mathcal{R}^C the complete energy R/T coefficient resulting from interactions of the ray under consideration with interfaces between S and R , and $T^G(R, S)$ the complete phase shift due to caustics along the ray between S and R . The relevant KMAH index in anisotropic media may also include a contribution at a point source S (if the slowness surface of the considered wave is concave at S). In isotropic media, this contribution is always zero.

The complete energy R/T coefficient \mathcal{R}^C , the relative geometrical spreading $\mathcal{L}(R, S)$ and the complete phase shift due to caustics are always reciprocal. Consequently, the elementary ray-theory elastodynamic Green function satisfies a very important property of reciprocity:

$$G_{in}(R, S, \omega) = G_{ni}(S, R, \omega) . \quad (59)$$

This relation is valid for any elementary seismic body wave generated by a point source.

For elementary ray-theory Green functions in inhomogeneous weakly anisotropic media see Pšenčík (1998).

Chaotic rays. Lyapunov exponents

In homogeneous media, geometrical spreading increases linearly with increasing length of the ray. In heterogeneous media, behaviour of geometrical spreading is more complicated, and depends considerably on the degree of heterogeneity of the medium. In models, in which heterogeneity exceeds certain degree, average geometrical spreading increases exponentially with increasing length of the ray. Rays in such a medium often exhibit chaotic behaviour, which is characterized by a strong sensitivity of rays to the initial ray data (for example, to ray parameters). The rays with only slightly differing ray data at an initial point tend to diverge *exponentially* at large distances from the initial point. Consequently, the rays intersect many times and many rays pass through the same point. With such *chaotic rays*, two-point ray tracing is practically impossible, and the ray tubes are not

narrow enough for travel time interpolation. The chaotic behaviour of rays increases with increasing length of rays and prevents applicability of the ray theory.

The exponential divergence of chaotic rays in the phase space (space formed by spatial coordinates x_i and slowness-vector components p_j) can be quantified by the so-called *Lyapunov exponents*. They may be introduced in several ways. It is common to express them in terms of characteristic values of the ray propagator matrix. The relevant expressions for the Lyapunov exponents and several numerical examples for 2D models without interfaces can be found in Klimeš (2002a). See also Červený et al. (2007), where other references can also be found.

The estimate of the Lyapunov exponent of a single finite ray depends on its position and direction. The Lyapunov exponents associated with rays of different positions and directions can be used to calculate *average Lyapunov exponents* for the model. The average Lyapunov exponents play a very important role in smoothing the models so that they are suitable for ray tracing (Červený et al. 2007).

Ray perturbation methods

Ray perturbation methods represent an important part of the ray theory. They can be used for approximate but fast and transparent solutions of forward problems in complicated models. They also play an important role in the inverse problems.

Ray perturbation methods are useful everywhere, where we wish to compute the wavefield or its constituents (travel times, amplitudes, polarization) in complicated models, which deviate only little from simple, *reference models*, for which computations are simpler. The solutions for complicated models are then sought as perturbations of simple solutions for the reference models. Examples are computations in weakly anisotropic media, which use an isotropic medium as reference, or in weakly dissipative media, which use a perfectly elastic medium as reference. Basic role in these approaches is played by *reference rays* traced in reference media. Solutions in perturbed media can be given in the form of a power series in the deviations of the perturbed and reference models. Mostly, the *first-order approximation*, i.e. the first term of the power series, is used.

The most frequent application of ray perturbation methods is, probably, in travel-time computations. First-order travel-time perturbation formulae for isotropic media are known and have been used (mostly in tomography) for several decades. Well known and broadly applied are also first-order travel-time formulae for anisotropic media (Červený and Jech, 1982; Hanyga, 1982; Červený, 2001, Sec.3.9). Travel-time perturbations are obtained by quadratures along reference rays. As an integration parameter, the parameter along reference rays is used.

Recently, several procedures for computation of higher-order travel-time perturbations were proposed. The procedure based on the so-called perturbation Hamiltonians (Klimeš, 2002b; Červený et al. 2007) allows computation of highly accurate travel times along a fixed reference ray in a reference medium. Another procedure is based on the so-called first-order ray tracing described briefly below. In the latter method, second-order travel-

time perturbations can be calculated along first-order rays.

Relatively recent is the use of ray perturbation methods in *first-order ray tracing* and *first-order dynamic ray tracing* (Pšenčík and Farra, 2007; Farra and Pšenčík, 2010). It allows to compute, approximately, not only rays and travel times, but whole wavefields. The idea of first-order ray tracing and dynamic ray tracing is simple. It is just sufficient to use eqs (25) and (40) with (21), in which the exact eigenvalue G_m is replaced by its first-order approximation. The resulting ray tracing provides first-order rays, first-order travel times and the first-order geometrical spreading. By simple quadratures along first-order rays, second-order travel-time corrections can be computed. This approach is applicable to P and S waves. In case of S waves, it can include the computation of coupling effects. First-order ray tracing and dynamic ray tracing are used in this case for computing common rays, first-order travel times and geometrical spreading along them, using the Hamiltonian (48). The wavefield of S waves is obtained by solving second-order coupling equations along the common rays. The procedure describes accurately S-wave propagation in isotropic media, and in anisotropic media when the S waves are coupled or even decoupled.

Procedure for computing the whole wave field is the *generalized Born scattering* (Chapman and Coates, 1994; Chapman, 2004). It is based on the first-order Born approximation, in which the exact Green function in the reference medium is replaced by the ray-theory Green function.

Ray perturbation method for weakly dissipative media

In viscoelastic media, the density-normalized stiffness tensor a_{ijkl} is complex valued:

$$a_{ijkl}(x_n) = a_{ijkl}^R(x_n) - ia_{ijkl}^I(x_n) . \quad (60)$$

If a_{ijkl}^I is small, the viscoelastic medium can be considered as a perturbation of a perfectly elastic medium (Červený, 2001, Sec.5.5.3). Reference ray in the reference perfectly elastic medium and corresponding real-valued travel time τ along the reference ray between points S and R can be obtained by standard ray tracing for perfectly elastic media. The imaginary travel time T^I (travel-time perturbation due to $-ia_{ijkl}^I$) can be then obtained by quadratures along the reference ray:

$$T^I = \frac{1}{2} \int_S^R Q^{-1}(\tau) d\tau . \quad (61)$$

The quantity Q in (61) is a direction-dependent *quality factor* for anisotropic media, corresponding to the Hamiltonian (21):

$$Q^{-1} = a_{ijkl}^I p_j p_l g_i g_k . \quad (62)$$

For general Hamiltonians, the quality factor Q is given by the relation $Q^{-1} = -\text{Im}\mathcal{H}(x_i, p_j)$.

The imaginary travel time T^I in (61) is responsible for the amplitude decay along the reference ray. For causal dissipation, the stiffness tensor (60) is frequency dependent. The

above described perturbation approach is then equivalent to the perturbation scheme, in which $a_{ijkl}^I(x_n, \omega)$ is considered to be of the order of ω^{-1} for $\omega \rightarrow \infty$ (Kravtsov and Orlov, 1990; Gajewski and Pšenčík, 1992).

In an inhomogeneous isotropic, weakly dissipative medium, the expression (62) reduces to the well-known formula

$$Q^{-1} = -2\text{Im}V/\text{Re}V, \quad (63)$$

in which V is the complex-valued velocity, $V = \alpha$ for P waves and $V = \beta$ for S waves. Complex-valued quantities α and β are generalizations (to the complex space) of real-valued α and β from (14).

Concluding remarks. Modifications and extensions of the ray method

In this review, we concentrated mainly on the forward applications of the zero-order ray approximation, particularly on the problems of computation of seismic body waves propagating in 3D layered, smoothly varying anisotropic or isotropic media containing smoothly curved structural interfaces. We have not discussed the applications of the ray method to the inverse problems (tomography, migration, etc.); our conclusions apply to these problems only indirectly.

The ray method is not valid universally. We have briefly described three serious limitations of the ray method: a) The ray method can be used only for high-frequency signals. b) In models, in which heterogeneity exceeds certain degree, the ray field has chaotic character, particularly at large distances from the source. c) The standard ray method cannot be used for computing S waves propagating in inhomogeneous, weakly anisotropic media. It must be replaced by the coupling ray theory. The coupling ray theory must be used even in moderately and strongly anisotropic media, in the vicinity of shear-wave singular directions.

The ray method fails, however, even in other singular situations. In smooth isotropic media, the most important type of singularity are *caustics*. Caustics may attain various forms. Various extensions of the ray method can be used to compute wavefields in caustic regions. These extensions are frequency dependent. See a detailed treatment of wavefields in caustic regions in Stamnes (1986) and also Kravtsov and Orlov (1999). In models with smooth structural interfaces, other singularities often appear. For edge and vertex points, see Ayzenberg et al. (2006). For critical singular regions, at which head waves separate from reflected waves, see Červený and Ravindra (1971). For the waves, whose rays are tangential to interfaces, see Thomson (1989).

Specific methods, designed for different types of singularities may be used for computing wavefields in singular regions. Disadvantage of these methods is that they are different for different singularities. Moreover, singular regions often overlap, and the wavefield in the overlapping region requires again different treatment. It is desirable to have available a more general extension of the ray method, applicable uniformly in any of the mentioned singular regions, or, at least, in most of them. Such an extension would simplify ray

computations considerably and could even lead to more accurate results.

Several such extensions of the ray method have been proposed. We do not describe them here in detail. Instead, we merely present references, in which more details and further references can be found. Let us mention the Maslov asymptotic ray theory introduced to seismology by Chapman and Drummond (1982), see also Thomson and Chapman (1985), Chapman (2004). Another extension of the ray method is based on the summation of Gaussian beams (Popov, 1982; Červený et al., 1982). For the relation of this method with the Maslov method see Klimeš (1984). The Gaussian beam summation method has found applications both in the forward modelling of seismic wavefields and in migrations in seismic exploration. It is closely related to the method of summation of Gaussian packets (Červený et al., 2007). For waves reflected from a smooth structural interface separating two heterogeneous, isotropic or anisotropic media, the Kirchhoff surface integral method can be used. For details and many references see Chapman (2004, Sec.10.4). Another useful extension of the ray method is the one-way wave equation approach (Thomson, 1999).

Bibliography

- Aki, K., and Richards, P., 1980. *Quantitative seismology*. San Francisco: W.H. Freeman & Co.
- Ayzenberg, M.A., Aizenberg, A.M., Helle, H.B., Klem-Musatov, K.D., Pajchel, J., and Ursin, B., 2007. 3D diffraction modeling of singly scattered acoustic wavefields based on the combination of surface integral propagators and transmission operators. *Geophysics*, 72: SM19–SM34.
- Babich, V.M., 1956. Ray method of the computation of the intensity of wave fronts (in Russian). *Dokl.Akad.Nauk SSSR*, 110: 355–357.
- Babich, V.M., 1961. Ray method of the computation of the intensity of wave fronts in elastic inhomogeneous anisotropic medium. In: Petrashen, G.I (ed.) Problems of the dynamic theory of propagation of seismic waves (in Russian), Vol. 5. Leningrad: Leningrad University Press, pp. 36–46. (Translation to English: *Geophys. J. Int.*, 118: 379–383, 1994.)
- Bakker, P.M., 1998. Phase shift at caustics along rays in anisotropic media. *Geophys. J. Int.*, 134: 515–518.
- Bakker, P.M., 2002. Coupled anisotropic shear-wave ray tracing in situations where associated slowness sheets are almost tangent. *Pure Appl. Geophys.*, 159: 1403–1417.
- Bulant, P., and Klimeš, L., 2002. Numerical algorithm of the coupling ray theory in weakly anisotropic media. *Pure Appl. Geophys.*, **159**, 1419–1435.
- Červený, V., 1972. Seismic rays and ray intensities in inhomogeneous anisotropic media. *Geophys. J. R. astr. Soc.*, 29: 1–13.

- Červený, V., and Jech, J., 1982. Linearized solutions of kinematic problems of seismic body waves in inhomogeneous slightly anisotropic media, *J. Geophys.*, 51: 96–104.
- Červený, V., 2001. *Seismic ray theory*. Cambridge: Cambridge University Press.
- Červený, V., and Ravindra, R., 1971. *Theory of seismic head waves*. Toronto: Toronto University Press.
- Červený, V., Klimeš, L., and Pšenčík, I., 1988. Complete seismic ray tracing in three-dimensional structures. In: Doornbos, D.J. (ed.) *Seismological algorithms*, New York: Academic Press, pp. 89–168.
- Červený, V., Klimeš, L., and Pšenčík, I., 2007. Seismic ray method: Recent developments. *Advances in Geophysics*, 48: 1–126 (<http://www.sciencedirect.com/science/bookseries/00652687>).
- Červený, V., Molotkov, I.A., and Pšenčík, I., 1977. *Ray method in seismology*. Praha: Univerzita Karlova.
- Červený, V., Popov, M.M., and Pšenčík, I., 1982. Computation of wave fields in inhomogeneous media. Gaussian beam approach. *Geophys. J.R. astr. Soc.*, 70: 109–128.
- Chapman, C.H., 2002. Seismic ray theory and finite frequency extensions. In: Lee, W.H.K., Kanamori, H., Jennings, P.C. (eds.), *International Handbook of Earthquake and Engineering Seismology, Part A*. New York: Academic Press, pp. 103–123.
- Chapman, C. H., 2004. *Fundamentals of seismic wave propagation*. Cambridge: Cambridge University Press.
- Chapman, C.H., and Coates, R.T., 1994. Generalized Born scattering in anisotropic media. *Wave Motion*, 19: 309–341.
- Chapman, C. H., and Drummond, R., 1982. Body-wave seismograms in inhomogeneous media using Maslov asymptotic theory. *Bull. seism. Soc. Am.*, 72: S277–S317.
- Coates, R.T., and Chapman, C.H., 1990. Quasi–shear wave coupling in weakly anisotropic 3-D media. *Geophys. J. Int.*, 103: 301–320.
- Farra, V., and Pšenčík, I., 2010. Coupled S waves in inhomogeneous weakly anisotropic media using first-order ray tracing. *Geophys. J. Int.*, 180: 405–417.
- Fedorov, F.I., 1968. *Theory of elastic waves in crystals*. New York: Plenum.
- Gajewski, D., and Pšenčík, I., 1992. Vector wavefield for weakly attenuating anisotropic media by the ray method. *Geophysics*, 57: 27–38.
- Gjøystdal, H., Iversen, E., Laurain, R., Lecomte, I., Vinje, V., and Åstebol, K., 2002. Review of ray theory applications in modelling and imaging of seismic data. *Stud. Geoph. Geod.*, 46: 113 - 164.

- Hanyga, A., 1982. The kinematic inverse problem for weakly laterally inhomogeneous anisotropic media, *Tectonophysics*, 90: 253–262.
- Jech, J., and Pšenčík, I., 1989. First-order perturbation method for anisotropic media. *Geophys. J. Int.*, 99: 369–376.
- Karal, F.C., and Keller, J.B., 1959. Elastic wave propagation in homogeneous and inhomogeneous media. *J. Acoust. Soc. Am.*, 31: 694–705.
- Klimeš, L., 1984. The relation between Gaussian beams and Maslov asymptotic theory. *Stud. Geophys. Geod.*, 28: 237–247.
- Klimeš, L., 2002a. Lyapunov exponents for 2-D ray tracing without interfaces. *Pure Appl. Geophys.*, 159: 1465–1485.
- Klimeš, L., 2002b. Second-order and higher-order perturbations of travel time in isotropic and anisotropic media. *Stud. Geophys. Geod.*, 46: 213–248.
- Klimeš, L., 2006. Common-ray tracing and dynamic ray tracing for S waves in a smooth elastic anisotropic medium. *Stud. Geophys. Geod.*, 50: 449–461.
- Klimeš, L., 2010. Phase shift of the Green tensor due to caustics in anisotropic media. *Stud. Geoph. Geod.*, 54: 269–289.
- Kravtsov, Yu.A., 1968. "Quasiisotropic" approximation to geometrical optics, *Dokl. AN SSSR*, 183, No.1: 74–77 (in Russian).
- Kravtsov, Yu.A., and Orlov, Yu.I., 1990. *Geometrical optics of inhomogeneous media*. Heidelberg: Springer Verlag.
- Kravtsov, Yu.A., and Orlov, Yu.I. 1999. *Caustics, catastrophes and wave fields*. Heidelberg: Springer Verlag.
- Popov, M.M., 1982. A new method of computation of wave fields using Gaussian beams. *Wave Motion*, 4, 85–97.
- Pšenčík, I., 1998. Green's functions for inhomogeneous weakly anisotropic media. *Geophys. J. Int.*, 135: 279–288.
- Pšenčík, I., and Farra, V., 2007. First-order P-wave ray synthetic seismograms in inhomogeneous weakly anisotropic media. *Geophys. J. Int.*, 170: 1243–1252.
- Stamnes, J.J., 1986. *Waves in focal regions*. Bristol: Adam Hilger.
- Thomson, C.J., 1989. Corrections for grazing rays to 2-D seismic modelling. *Geophys. J. Int.*, 96: 415–446.
- Thomson, C.J., 1999. The gap between seismic ray theory and full wavefield extrapolation. *Geophys. J. Int.*, 137: 364–380.
- Thomson, C. J., and Chapman, C. H., 1985. An introduction to Maslov's asymptotic method. *Geophys. J. R. astr. Soc.*, 83: 143–168.

Virieux, J., 1996. Seismic ray tracing. In: Boschi, E., Ekström, G., and Morelli, A. (eds.). Seismic modelling of Earth structures. Bologna: Editrice Compositori, pp. 223–304.