Geophysical Journal International

Geophys. J. Int. (2017) **210,** 561–569
Advance Access publication 2017 May 9
GJI Seismology

doi: 10.1093/gji/ggx183

Elementary Green function as an integral superposition of Gaussian beams in inhomogeneous anisotropic layered structures in Cartesian coordinates

Vlastislav Červený[1] and Ivan Pšenčík[2]

[1] *Faculty of Mathematics and Physics, Department of Geophysics, Charles University, Ke Karlovu* 3, 121 16 *Praha* 2, *Czech Republic*
[2] *Institute of Geophysics, Academy of Sciences of Czech Republic, Boční II,* 141 31 *Praha* 4, *Czech Republic. E-mail: ip@ig.cas.cz*

Accepted 2017 May 3. Received 2017 April 28; in original form 2016 September 30

SUMMARY

Integral superposition of Gaussian beams is a useful generalization of the standard ray theory. It removes some of the deficiencies of the ray theory like its failure to describe properly behaviour of waves in caustic regions. It also leads to a more efficient computation of seismic wavefields since it does not require the time-consuming two-point ray tracing. We present the formula for a high-frequency elementary Green function expressed in terms of the integral superposition of Gaussian beams for inhomogeneous, isotropic or anisotropic, layered structures, based on the dynamic ray tracing (DRT) in Cartesian coordinates. For the evaluation of the superposition formula, it is sufficient to solve the DRT in Cartesian coordinates just for the point-source initial conditions. Moreover, instead of seeking 3×3 paraxial matrices in Cartesian coordinates, it is sufficient to seek just 3×2 parts of these matrices. The presented formulae can be used for the computation of the elementary Green function corresponding to an arbitrary direct, multiply reflected/transmitted, unconverted or converted, independently propagating elementary wave of any of the three modes, P, S1 and S2. Receivers distributed along or in a vicinity of a target surface may be situated at an arbitrary part of the medium, including ray-theory shadow regions. The elementary Green function formula can be used as a basis for the computation of wavefields generated by various types of point sources (explosive, moment tensor).

Key words: Body waves; Seismic anisotropy; Theoretical seismology; Wave propagation.

1 INTRODUCTION

The method of integral superposition of Gaussian beams, correctly called paraxial Gaussian beams in order to distinguish them from exact Gaussian beams, is a powerful extension of the ray method. It removes several problems, which complicate applications of the ray method. The most important is the regular behaviour of wavefields evaluated by the superposition of Gaussian beams at caustics and their vicinities, where the ray method fails. The integral superposition of Gaussian beams does not provide entirely correct values in ray-theory shadow regions, but it guarantees a smooth transition from the illuminated to shadow region. This is in contrast with the ray method, which yields abrupt changes of the wavefield in this region. Computations of seismic wavefields based on the superposition of Gaussian beams do not require time-consuming two-point ray tracing, which is a basic part of every ray tracing code. The integral superposition of Gaussian beams can be evaluated at any point of the medium, including points in ray-theory shadow regions, without necessity to trace rays to these points.

The Gaussian beams are approximate, complex-valued solutions of the elastodynamic equation concentrated close to rays of seismic body waves. Thus, their traveltimes and amplitudes can be approximately evaluated not only along rays, as in the standard ray method, but also in their vicinities. Their frequency-dependent amplitudes decrease exponentially with the square of the distance from the ray in any plane intersecting the ray. This behaviour is a consequence of the use of the complex-valued matrix of spatial second-order derivatives of traveltime in the Taylor expansion of traveltime up to quadratic terms.

In this paper, we pay attention to the integral superposition of Gaussian beams, not to individual Gaussian beams. There is an extensive literature devoted to individual Gaussian beams propagating in inhomogeneous acoustic, isotropic or anisotropic media. For references, see, for example, Červený & Pšenčík (1983), Hanyga (1986), Červený (2001), Bleistein (2007), Kravtsov & Berczynski (2007), Červený & Pšenčík (2010) or Protasov (2015). The references to integral superposition (summation) of Gaussian beams are mostly devoted to acoustic or elastic isotropic inhomogeneous media, see Babich & Popov (1981), Červený *et al.* (1982), Popov (1982), Nowack & Aki (1984), Klimeš (1984), Červený (1985), George *et al.* (1987), White *et al.* (1987), Weber (1988), Červený *et al.* (2007), Vinje *et al.* (2008), and others. Explicit references

to integral superposition of Gaussian beams in inhomogeneous anisotropic media are difficult to find. Supperposition of Gaussian beams propagating in inhomogeneous isotropic and anisotropic media has been used in migration in seismic exploration, see, for example, Hill (1990, 2001), Alkhalifah (1995), Gray (2005), Zhu *et al.* (2007), Popov *et al.* (2010), Vinje *et al.* (2008), Gray & Bleistein (2009), Bleistein & Gray (2010), Protasov & Tcheverda (2012), Protasov (2015), Gao *et al.* (2017).

We start the derivation of the integral superposition formula from the superposition formula of Červený *et al.* (2007) in ray-centred coordinates. The formula was derived originally by Klimeš (1984) for a wavefield originating at an initial surface. We exploit the fact that the integral superposition of Červený *et al.* (2007) can be used not only for laterally varying, layered isotropic, but also anisotropic media.

Basic procedure in the computation of the elementary Green function as an integral superposition of Gaussian beams is the dynamic ray tracing (DRT), see again Červený *et al.* (2007). We call solutions of the DRT, which have a matrix form, paraxial matrices. In the following, we use the term *paraxial* to denote quantities obtained or related to the DRT. Useful property of paraxial solutions is that traveltime fields or wavefields constructed from them are independent of the used coordinate system. The DRT system, and, consequently, the expressions for the integral superposition of Gaussian beams, can be expressed in various coordinate systems, most often in ray-centred or Cartesian coordinate systems. The advantage of the use of the DRT in the ray-centred coordinates is the physical clarity of the concept and the low number of the DRT equations because the solution is sought in the form of 2×2 paraxial matrices. The disadvantage of such an approach is its relative complexity. The quantities in the ray-centred coordinates are computed in the coordinate system, which varies along the ray. In this respect, the straightforward use of the DRT in Cartesian coordinates is advantageous because the coordinate system, in which computations are performed, is fixed. Also, the structure of the right-hand sides of DRT equations in Cartesian coordinates is considerably simpler than in the ray-centred coordinates. As in ray-centred coordinates, the DRT in Cartesian coordinates is obtained by the differentiation of ray tracing equations with respect to ray parameters, see, for example, Červený (1972), Ralston (1983), Gajewski & Pšenčík (1990), Virieux & Farra (1991), Leung *et al.* (2007). This leads to a larger number of equations, from which the DRT consists. The solution of the DRT system in Cartesian coordinates can be formulated for different types of Hamiltonians. For example, Virieux & Farra (1991) or Leung *et al.* (2007), who deal with isotropic media, use Hamiltonian proposed by Burridge (1976), which is inhomogeneous in components p_i of the slowness vector $\mathbf{p}$, and has many advantages. Since it is, however, difficult to use a similar Hamiltonian in anisotropic media, we use a homogeneous Hamiltonian. The solution of the DRT in such a case has the form of 3×3 paraxial matrices. In this paper, we show that for the evaluation of the superposition formula for the elementary Green function, it is sufficient to seek the solution of the DRT in Cartesian coordinates in the form of only 3×2 paraxial matrices. We call such a DRT system the *reduced* DRT system. When identical initial conditions are used, the reduced DRT system yields the same results as the DRT system in ray-centred coordinates. Let us note that the reduced DRT system (Pšenčík & Teles, 1996) is currently used in the ANRAY program package (Gajewski & Pšenčík, 1990). The package ANRAY is freely available on the web pages of the SW3D Consortium Seismic Waves in Complex 3-D Structures (http://sw3d.cz).

The transformation of the superposition formula of Červený *et al.* (2007), which requires results of the DRT in ray-centred coordinates, into the formula requiring results of the reduced DRT in Cartesian coordinates represents an important contribution of this paper. We present superposition formula for the elementary Green function calculated along a ray of an elementary wave (direct, reflected/transmitted, converted, multiply reflected and converted, etc.) generated by a unit-force point source. The superposition formula thus represents an approximate expression for a high-frequency, *elementary Green function*. Elementary Green functions, which are related to elementary waves of the ray method, are useful in various applications in seismology and seismic exploration. The sum of elementary Green functions corresponding to various elementary waves then yields the high-frequency elastodynamic Green function. The elementary Green-function wavefield is considered intentionally. It can be used as a basis for the construction of any type of point sources (explosive, moment-tensor), and, using the representation theorem (Aki & Richards 1980), even for finite surface or finite volume sources.

In the main text, we explain the basic concepts, on which the computation of elementary Green function expressed as an integral superposition of Gaussian beams, is built. Auxiliary procedures like ray tracing and DRT are shifted to Appendices.

In Section 2, we present and discuss quantities, which can be obtained by solving two forms of DRT for inhomogeneous anisotropic layered media, one in ray-centred, and the other in Cartesian coordinates. We also describe there the computation of ray-theory elementary Green function amplitudes. Section 3 is devoted to the replacement of the quantities used in the formula for the integral superposition of Gaussian beams in inhomogeneous anisotropic media and obtained from the DRT in ray-centred coordinates by quantities obtained from the reduced DRT in Cartesian coordinates. In Section 4, some important concluding remarks are presented. Appendices A and B contain all the necessary equations for the ray tracing and DRT in inhomogeneous anisotropic media in Cartesian coordinates, respectively. The initial conditions at a point source for the ray tracing and DRT are included.

A specific role in this study is played by the following three points. One is the initial point S, at which the unit-force point source is situated, and from which ray tracing and DRT calculations start. Another point is the receiver R, at which the wavefield is evaluated by the summation of the contributions of nearby Gaussian beams. The contributions are extrapolated from the reference points P situated on rays Ω, along which Gaussian beam contributions are calculated. The points P should be chosen so that the receiver R is situated in their close, paraxial, vicinity. In this contribution, we choose points P as points of intersection of rays Ω with a smooth surface called a *target surface*. Target surface is a smooth surface, on which rays Ω terminate. The target surface may, but need not, represent a structural surface (interface, free surface). For the evaluation of the integral superposition, it is convenient if arriving rays are close to perpendicular to the target surface. In principle, one can choose a different target surface for each computed elementary Green function at each receiver R. On the other hand, one may use a common target surface for all considered receivers R and all computed elementary Green functions. The receiver R may be situated on the target surface or close to it. The points S and P situated on the rays Ω can be specified either by their Cartesian coordinates or by a variable parameter along the ray. Since we use the traveltime τ as the variable parameter along the ray, we use either x_m^S or τ_0 for the specification of the point S, and x_m^P or τ for the points P.

The receiver R is specified by its Cartesian coordinates x_m^R. The ray passing directly through the receiver R is not required.

In this paper, we do not consider situations, in which receivers R are distributed inside a volume. For such a kind of problems it is more convenient to use the superposition of Gaussian packets than Gaussian beams, see, for example Klimeš (2014a).

To express the equations in 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 ($i, j, k, \ldots$) the values 1, 2, or 3. The Einstein summation convention is used throughout the paper. The matrices and vectors are denoted by bold upright symbols. The DRT is used here in two coordinate systems, namely in ray-centred coordinates q_i and in Cartesian coordinates x_i. To distinguish the matrices in ray-centred coordinates q_i from the analogous matrices in Cartesian coordinates x_i, we use superscripts (q) and (x) over them. Further, to distinguish between 2×2 and 3×3 matrices, we use the circumflex (ˆ) above symbols for 3×3 matrices. The vectors are considered as column matrices. Whenever there may be reason for confusion, the dimensions of the matrices are explicitly indicated.

2 RAY THEORY FOR INHOMOGENEOUS ANISOTROPIC LAYERED STRUCTURES

In this section, we discuss results of two formulations of the DRT and describe the evaluation of the ray-theory complex-valued amplitudes of separate elementary body waves generated by a unit-force point source, and propagating in inhomogeneous anisotropic layered structures. We start with the presentation of expressions in ray-centred coordinates since they represent an important available basis for the derivations of formulae in Cartesian coordinates. We skip detailed derivation and discussion of basic formulae of the ray method. They can be found in Červený (2001).

In the following, we consider a ray Ω, specified by two ray parameters γ_1, γ_2. They may be, for example, the take-off angles of the ray Ω or two components of the slowness vector of the ray Ω at the point source S. Ray tracing equations and the corresponding initial conditions can be found in Appendix A. The reduced DRT equations in Cartesian coordinates with the corresponding initial conditions are given in Appendix B.

2.1 Dynamic ray tracing

The ray-tracing equations can be used to compute necessary quantities only on the considered ray Ω, not in its vicinity. This is, however, not sufficient for the calculation of the ray-theory amplitudes and/or Gaussian beams concentrated to ray Ω. This is because the ray-theory amplitudes depend on geometrical spreading, which is related to the ray field, not to a single ray. In the case of Gaussian beams, we also need to compute complex-valued paraxial traveltimes (the complex-valued traveltimes in the vicinity of the ray Ω). For the computation of the quantities related to the ray field, it is necessary to compute system of rays around Ω or to supplement the ray tracing by an additional procedure called DRT.

DRT is a basic procedure for the computation of geometrical spreading and for the computation of the second derivatives of the traveltime field with respect to the used coordinates, along the ray. Geometrical spreading is a basic quantity in the computation of the ray-theory amplitudes along the ray. Therefore, we speak of DRT in order to distinguish it from the standard (kinematic) ray tracing, which provides kinematic quantities. DRT 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 ray tracing, or along an already known ray Ω.

The DRT system can be expressed in various coordinate systems (Cartesian x_i, ray-centred q_i, etc.). The DRT system in ray-centred coordinates designed for the computation of Gaussian beams was described in detail in Červený & Pšenčík (2010). In this paper, we briefly review the DRT system in ray-centred coordinates q_i, and introduce the reduced DRT in Cartesian coordinates, in which the 3×2 matrices instead of 3×3 paraxial matrices are considered.

2.1.1 *Dynamic ray tracing in ray-centred coordinates*

In the ray-centred coordinates q_i, the selected ray Ω represents its coordinate axis q_3. The coordinate axes q_1 and q_2 are usually introduced as mutually perpendicular straight lines situated in the plane tangent to the wave front, with the origin at the intersection of the wave front with the ray Ω. The transformation from ray-centred to Cartesian coordinates and vice versa is controlled by the 3×3 transformation matrices $\hat{\mathbf{H}}(\tau)$ and $\hat{\overline{\mathbf{H}}}(\tau)$ with elements:

$$H_{im}(\tau) = \partial x_i / \partial q_m \ , \quad \overline{H}_{im}(\tau) = \partial q_i / \partial x_m \ . \tag{1}$$

The transformation matrices have several useful properties. First of all, $\hat{\mathbf{H}} \cdot \hat{\overline{\mathbf{H}}} = \hat{\mathbf{I}}$, where $\hat{\mathbf{I}}$ is the 3×3 identity matrix. Further, $H_{i3} = \mathcal{U}_i$ and $H_{3i} = p_i$, where $\boldsymbol{\mathcal{U}}$ is the ray-velocity vector and $\mathbf{p}$ is the slowness vector, both known from ray tracing, see Appendix A. One of the column vectors of the transformation matrix $\hat{\mathbf{H}}$, with elements H_{i1} or H_{i2}, can be determined by solving an ordinary differential equation of the first order

$$dH_{iK}(\tau)/d\tau = -H_{mK}(\tau)\eta_m(\tau)p_i(\tau)/[p_n(\tau)p_n(\tau)] \tag{2}$$

along the ray Ω. Here $\eta_i = dp_i/d\tau$ is known from kinematic ray tracing, see eq. (A7). The other of the above two column vectors of the matrix $\hat{\mathbf{H}}$ can be determined from the condition of orthogonality of the columns of the matrix $\hat{\mathbf{H}}$. For more details and the description how to evaluate the transformation matrices $\hat{\mathbf{H}}$ and $\hat{\overline{\mathbf{H}}}$, see Červený & Pšenčík (2010, section 2.3).

The DRT in ray-centred coordinates is used to determine two 2×2 matrices $\mathbf{Q}^{(q)}(\tau)$ and $\mathbf{P}^{(q)}(\tau)$, with elements

$$Q_{IJ}^{(q)}(\tau) = \partial q_I / \partial \gamma_J \ , \quad P_{IJ}^{(q)}(\tau) = \partial p_I^{(q)} / \partial \gamma_J \ . \tag{3}$$

The parameters γ_J may be again specified as the ray parameters.

From the 2×2 paraxial matrices $\mathbf{Q}^{(q)}(\tau)$ and $\mathbf{P}^{(q)}(\tau)$, we can obtain the important 2×2 matrix $\mathbf{M}^{(q)}(\tau)$ of the second derivatives of traveltime field T with respect to ray-centred coordinates q_1 and q_2, whose elements have the form:

$$M_{IJ}^{(q)}(\tau) = \partial^2 T / \partial q_I \partial q_J \ . \tag{4}$$

The 2×2 symmetric matrix $\mathbf{M}^{(q)}(\tau)$, with three independent elements $M_{IJ}^{(q)}(\tau)$, can be expressed in terms of $\mathbf{Q}^{(q)}(\tau)$ and $\mathbf{P}^{(q)}(\tau)$. As

$$M_{IJ}^{(q)}(\tau) Q_{JK}^{(q)}(\tau) = \frac{\partial^2 T}{\partial q_I \partial q_J} \frac{\partial q_J}{\partial \gamma_K} = \frac{\partial p_I^{(q)}}{\partial q_J} \frac{\partial q_J}{\partial \gamma_K} = \frac{\partial p_I^{(q)}}{\partial \gamma_K} = P_{IK}^{(q)}(\tau), \tag{5}$$

we obtain

$$\mathbf{M}^{(q)}(\tau) = \mathbf{P}^{(q)}(\tau)(\mathbf{Q}^{(q)}(\tau))^{-1} \ . \tag{6}$$

2.1.2 Reduced DRT in Cartesian coordinates

The disadvantage of the DRT system in the ray-centred coordinates with respect to the DRT in Cartesian coordinates is that the DRT system in ray-centred coordinates is more complicated than in Cartesian coordinates. It is because we have to rotate appropriately the whole system at any step of the computation. The disadvantage of the DRT system in Cartesian coordinates is a larger number of its equations. We can, however, reduce the number of equations of the DRT in Cartesian coordinates and compute only the first two columns of 3×3 paraxial matrices $\hat{\mathbf{Q}}^{(x)}(\tau)$ and $\hat{\mathbf{P}}^{(x)}(\tau)$, namely the elements $Q_{iJ}^{(x)}(\tau)$ and $P_{iJ}^{(x)}(\tau)$, see, for example, Gajewski & Pšenčík (1990), Pšenčík & Teles (1996). These four columns are sufficient for the computation of Gaussian beams at any point of the ray Ω.

The elements $Q_{iJ}^{(x)}(\tau)$ and $P_{iJ}^{(x)}(\tau)$ of 3×3 paraxial matrices $\hat{\mathbf{Q}}^{(x)}(\tau)$ and $\hat{\mathbf{P}}^{(x)}(\tau)$ read

$$Q_{iJ}^{(x)}(\tau) = \partial x_i / \partial \gamma_J \,, \quad P_{iJ}^{(x)}(\tau) = \partial p_i / \partial \gamma_J \,. \tag{7}$$

Here, p_i are again Cartesian components of the slowness vector $\mathbf{p}$ and γ_J are ray parameters specifying the ray Ω. The elements $Q_{iJ}^{(x)}(\tau)$ and $P_{iJ}^{(x)}(\tau)$ are the solution of the reduced DRT system (B1). They must satisfy the constraint relation (B4).

2.2 Ray-theory complex-valued amplitudes

Let us again consider a harmonic, elementary high-frequency seismic body wave propagating in a laterally varying, anisotropic layered structure and the ray Ω corresponding to this wave. We consider that the wavefield is generated by a unit-force point source located at the point S, that is, we consider the elementary Green-function wavefield. For the references, see, for example Kendall *et al.* (1992), Pšenčík & Teles (1996), Červený (2001), Červený *et al.* (2007), Klimeš (2012). At a point P, arbitrarily chosen on the ray Ω, the wavefield is represented by the zero-order ray approximation of the elementary Green-function displacement tensor with Cartesian components $u_{ij}(P)$:

$$\begin{aligned} u_{ij}(P) &= U_{ij}(P) \exp[-\mathrm{i}\omega(t - T(P))] \\ &= A(P) g_i(P) g_j(S) \exp[-\mathrm{i}\omega(t - T(P))]. \end{aligned} \tag{8}$$

The symbol $U_{ij}(P)$ denotes Cartesian components of the tensorial zero-order ray-theory amplitude, $A(P)$ is the corresponding scalar zero-order ray-theory amplitude. The amplitude $A(P)$ can be, in general, complex-valued. The symbols $g_i(P)$ and $g_j(S)$ denote Cartesian components of the real-valued polarization vectors $\mathbf{g}$ specified at points P and S, respectively. $T(P)$ is the traveltime at the point P of the ray Ω. Due to the homogeneity of the considered Hamiltonian (A4), $T(P) = \tau(P)$, where τ is the parameter along the ray Ω with the meaning of traveltime. The traveltime $T(P)$ and the polarization vectors $\mathbf{g}(S)$ and $\mathbf{g}(P)$ are determined during the ray tracing. It remains to discuss the computation of the scalar ray-theory amplitude $A(P)$. For this, results of the DRT are required.

The scalar ray-theory amplitude $A(P)$ of the elementary Green function can be expressed as:

$$A(P) = \frac{\mathcal{R}^C(P, S) \exp[\mathrm{i} T^G(P, S)]}{4\pi [\rho(P)\rho(S) C(P) C(S)]^{1/2} \mathcal{L}(P, S)} \,, \tag{9}$$

see Červený *et al.* (2007, eq. 78). In eq. (9), ρ is the density, $\mathcal{C}$ the phase velocity (known from ray tracing). The symbol $\mathcal{R}^C(P, S)$ denotes the product of all normalized energy reflection/transmission coefficients along ray Ω from S to P. For its detailed description, see Červený (2001, section 5.4.4). The function $T^G(P, S)$ in (9) is the complete phase shift due to caustics along the ray from the source S to the point P. It is related to the so-called KMAH index. The possible phase shift directly at the point source in anisotropic media is included in $T^G(P, S)$. For details and computation of the phase shift due to caustics in anisotropic media, see Bakker (1998), Garmany (2001) and Klimeš (2010, 2014b). The function $\mathcal{L}(P, S)$ is the relative geometrical spreading defined as:

$$\mathcal{L}(P, S) = |\det \mathbf{Q}_{\mathcal{L}}^{(q)}(P, S)|^{1/2} \,, \tag{10}$$

where the 2×2 matrix $\mathbf{Q}_{\mathcal{L}}^{(q)}(P, S)$ is the solution $\mathbf{Q}^{(q)}(P)$ of the DRT in ray-centred coordinates with the initial conditions $\mathbf{Q}^{(q)}(S) = \mathbf{0}$ and $\mathbf{P}^{(q)}(S) = \mathbf{I}$, see Červený (2001, eq. (4.10.11)). The symbols $\mathbf{0}$ and $\mathbf{I}$ denote the 2×2 null and identity matrices, respectively. The subscript $\mathcal{L}$ of the matrix $\mathbf{Q}_{\mathcal{L}}^{(q)}(P, S)$ indicates the special initial conditions used for its generation. Eq. (10) can be simply generalized for the initial conditions $\mathbf{Q}^{(q)}(S) = \mathbf{0}$, $\mathbf{P}^{(q)}(S) = \mathbf{P}_0^{(q)}$, where $\mathbf{P}_0^{(q)}$ is an arbitrary finite and non-zero 2×2 matrix. Since the DRT is linear, the DRT solution for the new initial conditions, obtained by the multiplication of the original ones by a constant matrix, is the original solution multiplied by this constant matrix. Thus, the multiplication of the initial conditions used for the generation of $\mathbf{Q}_{\mathcal{L}}^{(q)}(P, S)$ by $\mathbf{P}_0^{(q)}$ yields $\mathbf{Q}^{(q)}(P) = \mathbf{Q}_{\mathcal{L}}^{(q)}(P, S)\mathbf{P}_0^{(q)}$. It is then easy to generalize eq. (10) to:

$$\mathcal{L}(P, S) = \left[\frac{|\det \mathbf{Q}^{(q)}(P)|}{|\det \mathbf{P}^{(q)}(S)|} \right]^{1/2} \,. \tag{11}$$

The expressions for the scalar ray-theory amplitude $A(P)$ can be now written as:

$$A(P) = \overline{A}(P) \left[\frac{|\det \mathbf{P}^{(q)}(S)|}{|\det \mathbf{Q}^{(q)}(P)|} \right]^{1/2} = \frac{\overline{A}(P)}{\mathcal{L}(P, S)} \,. \tag{12}$$

Here $\overline{A}(P)$ is the spreading-free scalar ray-theory amplitude, which is given by the relation:

$$\overline{A}(P) = \frac{\mathcal{R}^C(P, S) \exp[\mathrm{i} T^G(P, S)]}{4\pi [\rho(S)\rho(P) C(S) C(P)]^{1/2}} \,. \tag{13}$$

Let us emphasize that $A(P)$ is singular at caustic points, where $|\det \mathbf{Q}^{(q)}(P)|^{1/2} = 0$, and thus $\mathcal{L}(P, S) = 0$. But $\overline{A}(P)$ is regular there.

Throughout this section, we considered the point P situated in smooth parts of a medium, not on structural interfaces or the Earth's surface. If the point P is situated on such a surface, it is necessary to consider not only the incident wavefield characterized here by the zero-order ray approximation of the elementary Green-function displacement tensor $u_{ij}(P)$ given in eq. (8), but also the wavefields generated at the corresponding surface. To take this into account, one must replace the polarization vector $\mathbf{g}(P)$ by the so-called *conversion vector*. For the conversion vector for the free surface, see Gajewski & Pšenčík (1987). The conversion vector consists of the polarization vector $\mathbf{g}(P)$ of the incident wave, supplemented by the sum of polarization vectors of all generated waves, each of which is multiplied by the appropriate *displacement* free-surface reflection coefficient. For the relations between normalized energy reflection/transmission coefficients and displacement reflection/transmission coefficients, see Červený (2001, section 5.4.4).

3 TIME-HARMONIC ELEMENTARY GREEN FUNCTION AS AN INTEGRAL SUPERPOSITION OF GAUSSIAN BEAMS

In Section 3.1, we introduce the formula for the time-harmonic elementary Green function for inhomogeneous anisotropic layered structures expressed in terms of Gaussian beam integral superposition. The formula depends on quantities whose evaluation requires DRT in ray-centred coordinates. In Section 3.2, we show how to calculate these DRT quantities using the reduced DRT in Cartesian coordinates. Finally, in Section 3.3, we summarize the evaluation of the elementary Green function as an integral superposition of Gaussian beams with the help of the reduced DRT in Cartesian coordinates.

3.1 Elementary Green function as an integral superposition of Gaussian beams in ray-centred coordinates

The expression for Gaussian beam integral superposition of elementary Green function in 3-D inhomogeneous isotropic media was first derived by Klimeš (1984, eq. (77)). Here we use it in the form given in eq. (169) of Červený *et al.* (2007). The expression, whose important elements are specified in the ray-centred coordinates, can be used not only in inhomogeneous isotropic, but also in inhomogeneous anisotropic media. In the notation adopted in this paper, the expression for the elementary Green function in 3-D media expressed as an integral superposition of Gaussian beams $u^B_{ij}(R,\omega)$ reads:

$$u^B_{ij}(R,\omega) = (\omega/2\pi) \iint_{\mathcal{D}} \mathrm{d}\gamma_1 \mathrm{d}\gamma_2 U_{ij}(P) |\det \mathbf{Q}^{(q)}(P)| \times \{-\det[\mathbf{M}^{(q)}(P) - \mathbf{M}(P)]\}^{1/2} \exp[\mathrm{i}\omega\theta(R,P)], \quad (14)$$

where the argument of $\{-\det[\mathbf{M}^{(q)}(P) - \mathbf{M}(P)]\}^{1/2}$ is chosen so that it satisfies the relation

$$\mathrm{Re}\{-\det[\mathbf{M}^{(q)}(P) - \mathbf{M}(P)]\}^{1/2} > 0 \quad \text{for } \mathrm{Im}[\mathbf{M}^{(q)}(P) - \mathbf{M}(P)] \neq 0. \quad (15)$$

The symbol $U_{ij}(P)$ denotes the Cartesian component of the tensorial zero-order ray-theory amplitude (8). $\mathbf{M}^{(q)}(P)$ is the 2×2 real-valued matrix (6) of the second derivatives of traveltime with respect to ray-centred coordinates q_I. It can be obtained from the DRT in ray-centred coordinates. The function $\theta(R,P)$ is given by the relation:

$$\theta(R,P) = \tau(P) + \left(x^R_k - x^P_k\right) p_k(P) + \frac{1}{2}\left(x^R_k - x^P_k\right) \mathcal{M}_{kl}(P) \left(x^R_l - x^P_l\right). \quad (16)$$

Here P denotes a point on the ray Ω with coordinates x^P_m, close to the receiver R. The quantity $\tau(P)$ is the real-valued traveltime at P, measured along Ω from the initial point S, and $p_k(P)$ is the k-th Cartesian component of the real-valued slowness vector $\mathbf{p}$ at the point P. The 3×3 complex-valued matrix $\hat{\boldsymbol{\mathcal{M}}}(P)$ is related to the 2×2 complex-valued matrix $\mathbf{M}(P)$ of parameters of Gaussian beams, which controls the shape of Gaussian beam (mainly its width) along the ray Ω. The matrix $\mathbf{M}(P)$ satisfies the existence conditions of Gaussian beams, that is, it is finite, symmetric and its imaginary part is positively definite. Otherwise, it can be chosen arbitrarily. It varies along the ray Ω, and can be recalculated from one point of the ray Ω to another using an appropriate DRT in ray-centred coordinates. If $\mathbf{M}$ satisfies the existence conditions at one point of the ray Ω, then it satisfies them at any point of the ray Ω, see section 4 of Červený & Pšenčík (2010). For more details on the choice and optimization of the parameters of Gaussian beams expressed in terms of matrix $\mathbf{M}(P)$ see Klimeš (1989).

The relation of the 3×3 complex-valued matrix $\hat{\boldsymbol{\mathcal{M}}}(P)$ to the 2×2 complex-valued matrix $\mathbf{M}(P)$ of the parameters of Gaussian beams is given by the relation derived by Červený & Klimeš (2010):

$$\mathcal{M}_{ij} = \bar{H}_{Ji} M_{JK} \bar{H}_{Kj} + p_i \eta_j + \eta_i p_j - p_i p_j \mathcal{U}_k p_k \,. \quad (17)$$

The real-valued quantities p_i, η_i and $\mathcal{U}_i$ are Cartesian components of the slowness, eta and ray-velocity vectors, respectively, which are known from ray tracing.

In eq. (14), R is again the receiver point with coordinates x^R_m, P is the reference point with coordinates x^P_m, situated on the ray Ω, specified by ray parameters γ_1, γ_2. The reference point P should be chosen so that the receiver R is situated in its paraxial vicinity. In this paper, we specify the reference point P as the point of intersection of the ray Ω with the arbitrarily chosen *target surface* Σ^{tar}. The target surface is a smooth surface passing through the receiver R or close to it.

For each ray specified by ray parameters γ_1, γ_2 in the integral superposition (14), the relevant Gaussian beam is concentrated to this ray, and vanishes at some distance from it. The region of the integration $\mathcal{D} = \mathcal{D}(\gamma_1, \gamma_2)$ in (14) represents the region in the ray-parameter domain, for which the value of the integrand on the target surface Σ^{tar} is greater than a prescribed threshold.

Let us rewrite the integral (14) into the form convenient for further transformations. We denote

$$|\det \mathbf{Q}^{(q)}(P)|\{-\det[\mathbf{M}^{(q)}(P) - \mathbf{M}(P)]\}^{1/2} = |\det \mathbf{Q}^{(q)}(P)|^{1/2}[-\det \boldsymbol{\mathcal{N}}(P)]^{1/2}, \quad (18)$$

where the 2×2 complex-valued matrix $\boldsymbol{\mathcal{N}}(P)$ is given by the relation

$$\boldsymbol{\mathcal{N}}(P) = \mathbf{P}^{(q)}(P) - \mathbf{M}(P)\mathbf{Q}^{(q)}(P). \quad (19)$$

Note that the factor $|\det \mathbf{Q}^{(q)}(P)|^{1/2}$ on the right-hand side of (18) cancels the factor $|\det \mathbf{Q}^{(q)}(P)|^{1/2}$ appearing in the denominator of the scalar zero-order ray-theory amplitude $A(P)$, which enters the tensorial zero-order ray amplitude $U_{ij}(P)$ in eq. (12). This removes the singularity caused by the above factor when it vanishes. Consequently the integrand of (14) is always regular, even at caustics. This is a significant difference of the integral superposition (14) of Gaussian beams with respect to the standard ray-theory, in which amplitudes rise to infinity when $|\det \mathbf{Q}^{(q)}(P)|^{1/2}$ approaches zero. The integral superposition of Gaussian beams for the elementary Green-function wavefield in ray-centred coordinates can be rewritten into the following form:

$$u^B_{ij}(R,\omega) = (\omega/2\pi) \iint_{\mathcal{D}} \mathrm{d}\gamma_1 \mathrm{d}\gamma_2 \overline{A}(P) g_i(P) g_j(S) |\det \mathbf{P}^{(q)}(S)|^{1/2} \times [-\det \boldsymbol{\mathcal{N}}(P)]^{1/2} \exp[\mathrm{i}\omega\theta(R,P)]. \quad (20)$$

The argument of $[-\det \boldsymbol{\mathcal{N}}(P)]^{1/2}$ is again chosen so that it satisfies relation (15). The symbol $\overline{A}(P)$ in (20) is given in (13). Note that it also involves the complete phase shift due to caustics $T^G(P,S)$. The symbol $\boldsymbol{\mathcal{N}}(P)$ is given in (19) and $\theta(R,P)$ in (16). For $\mathbf{P}^{(q)}(S)$, see the text before eq. (11). The reference points P with Cartesian coordinates x^P_m are situated at intersections of rays, specified by the ray parameters γ_1, γ_2, with the target surface Σ^{tar}.

3.2 Evaluation of the elementary Green function from the results of the reduced DRT in Cartesian coordinates

In this section, we derive formulae for the elementary Green function expressed as an integral superposition of Gaussian beams from the results of the reduced DRT in Cartesian coordinates, see Section 2.1.2 and Appendix B. The reduced DRT provides elements $Q_{iN}^{(x)} = \partial x_i/\partial\gamma_N$ and $P_{iN}^{(x)} = \partial p_i/\partial\gamma_N$ of paraxial matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ along the ray specified by ray parameters γ_1, γ_2. The 3×2 matrices with elements $Q_{iN}^{(x)}$ and $P_{iN}^{(x)}$ are sufficient for our purpose. The complete 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ with elements $Q_{ij}^{(x)} = \partial x_i/\partial\gamma_j$ and $P_{ij}^{(x)} = \partial p_i/\partial\gamma_j$, respectively, are not required.

If we wish to evaluate the integral superposition (20) using the solution of the reduced DRT in Cartesian coordinates, we need to express the matrices $\mathbf{Q}^{(q)}$, $\mathbf{P}^{(q)}$ and $\boldsymbol{\mathcal{N}}$ in terms of the solution of the reduced DRT. In the following, we use equations derived by Klimeš (1994). In contrast to Klimeš (1994), we use only elements $Q_{iJ}^{(x)}$ and $P_{iJ}^{(x)}$ of 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$. For $Q_{iK}^{(q)} = \partial q_i/\partial\gamma_K$ we simply get

$$Q_{iK}^{(q)} = \overline{H}_{ij} Q_{jK}^{(x)} , \tag{21}$$

where $\overline{H}_{ij}$ are elements of the transformation matrix $\hat{\overline{\mathbf{H}}}$, given in eq. (1). The derivation of transformation relation for $P_{IK}^{(q)} = \partial p_I^{(q)}/\partial\gamma_K$ is slightly more complicated, and yields:

$$P_{IK}^{(q)} = H_{mI} P_{mK}^{(x)} + F_{Ij} \overline{H}_{jK} . \tag{22}$$

Here H_{iJ} are elements of the transformation matrix $\hat{\mathbf{H}}$, given in eq. (1). The elements F_{mn} of the 3×3 matrix $\hat{\mathbf{F}}$ have the form:

$$F_{mn} = p_k \frac{\partial^2 x_k}{\partial q_m \partial q_n} . \tag{23}$$

Klimeš (1994, eq. 36) proved that

$$F_{MN} = 0, \quad F_{I3} = -H_{iI}\eta_i . \tag{24}$$

Inserting (24) into (22) yields the final transformation relation between $P_{IJ}^{(q)}$ obtained from the DRT in ray-centred coordinates and $P_{iJ}^{(x)}$ and $Q_{iJ}^{(x)}$ obtained from the reduced DRT in Cartesian coordinates:

$$P_{IK}^{(q)} = H_{mI} \left(P_{mK}^{(x)} - \eta_m p_j Q_{jK}^{(x)} \right) . \tag{25}$$

Use of eqs (21) and (25) in eq. (19) makes possible to express $\mathcal{N}_{IJ}$ in terms of quantities obtained from the reduced DRT in Cartesian coordinates:

$$\overline{\mathcal{N}}_{IJ} = H_{mI} \left(P_{mJ}^{(x)} - \eta_m p_j Q_{jJ}^{(x)} \right) - M_{IL} \overline{H}_{Lj} Q_{jJ}^{(x)} . \tag{26}$$

The bar over the elements of the matrix $\boldsymbol{\mathcal{N}}$ in eq. (26) is used to indicate that $\overline{\boldsymbol{\mathcal{N}}}$ is expressed in terms of quantities obtained from the reduced DRT in Cartesian coordinates. It is important to emphasize that the 2×2 matrix $\mathbf{M}$ of parameters of Gaussian beams in eq. (26) is considered to be specified at the same point of the ray as the other quantities in eq. (26), see the discussion below.

3.3 Elementary Green function as a Gaussian beam integral superposition in Cartesian coordinates

Results of the preceding section can be used in the transformation of the integral superposition formula (20) to Cartesian coordinates. We take into account that for the 2×2 matrix $\mathbf{P}^{(q)}(S)$ required in eq. (20), eq. (25) yields:

$$P_{IK}^{(q)}(S) = H_{mI}(S) P_{mK}^{(x)}(S) \tag{27}$$

because $Q_{iJ}^{(x)}(S) = 0$ at a point source. Inserting eqs (26) and (27) into (20), we arrive at the final expression for the Gaussian beam integral superposition of the elementary Green function in Cartesian coordinates:

$$u_{ij}^B(R,\omega) = (\omega/2\pi) \iint_{\mathcal{D}} \mathrm{d}\gamma_1 \mathrm{d}\gamma_2 \overline{A}(P) g_i(P) g_j(S) \times |\det[\mathbf{H}^T(S)\mathbf{P}^{(x)}(S)]|^{1/2} [-\det \overline{\boldsymbol{\mathcal{N}}}(P)]^{1/2} \exp[\mathrm{i}\omega\theta(R,P)] . \tag{28}$$

The argument of $[-\det \overline{\boldsymbol{\mathcal{N}}}(P)]^{1/2}$ is again chosen so that it satisfies relation (15).

All the quantities in (28) can be obtained from ray tracing and reduced DRT in Cartesian coordinates. In eq. (28), $\overline{A}(P)$ is given in (13), $g_i(P)$ and $g_j(S)$ are Cartesian components of the real-valued polarization vectors specified at points P and S, respectively. If the point P is situated on a structural interface or on the Earth's surface, the polarization vector $\mathbf{g}(P)$ must be replaced by the conversion vector as described in Section 2.2. The elements of the matrix $\overline{\boldsymbol{\mathcal{N}}}(P)$ are given in eq. (26). The function $\theta(R, P)$ is given in eq. (16). For the evaluation of the integral superposition (28), we also need to know the transformation matrices $\hat{\mathbf{H}}$ and $\hat{\overline{\mathbf{H}}}$. They can be determined by solving the ordinary differential eq. (2) and from the relations described around eq. (2). The Gaussian beam integral superposition of elementary Green function (28) is regular everywhere, including caustics.

Let us briefly discuss the 2×2 matrix of Gaussian beam parameters $\mathbf{M}$, which appears in $\overline{\boldsymbol{\mathcal{N}}}(P)$ in eq. (28) and also enters it through the matrix $\boldsymbol{\mathcal{M}}(P)$, see eq. (16). The matrix $\mathbf{M}$ is specified at the reference points P. In principle, it could be specified at any point of the ray Ω. A typical option is to specify it at the initial point S of the ray Ω. For the transformation of the matrix $\mathbf{M}$ from the point S to the point P, it would be necessary to seek an additional solution of the reduced DRT in Cartesian coordinates to calculate the propagator matrix and use it for the transformation of $\mathbf{M}(S)$ to $\mathbf{M}(P)$. It is, therefore, preferable to specify the matrix of Gaussian beam parameters at the point P.

For the evaluation of the time-domain version of elementary Green function from the frequency domain formula (28) at the point R , it is necessary to compute the expression under the integral for a series of frequencies ω_k, $k = 1, 2, \ldots$, with $\Delta\omega = \omega_{k+1} - \omega_k = \text{const}$. In this case, it is recommended to use the fast frequency algorithm, see Červený (2001, section 6.1.7), in which $\exp[\mathrm{i}\omega_k\theta(\mathrm{R},\mathrm{P})] = \exp[\mathrm{i}\omega_1\theta(\mathrm{R},\mathrm{P})]\mathrm{A}^{k-1}$, where $A = [\mathrm{i}\Delta\omega\theta(\mathrm{R},\mathrm{P})]$.

4 CONCLUDING REMARKS

Here we present several additional remarks and comments to the presented equations for the Gaussian beam integral superposition of an elementary Green function in inhomogeneous anisotropic layered structures in Cartesian coordinates.

Integral superposition proposed in this paper has the following advantages:

(1) All computations, including DRT, are performed in Cartesian coordinates. Similarly, the positions of the initial point S of the ray (a point source), of the receiver point R and of the points P of the intersection of rays with the target surface Σ^{tar} are specified in Cartesian coordinates.

(2) It is sufficient to use only the reduced version of the DRT in Cartesian coordinates described in Section 2.1.2, and compute only elements $Q_{iJ}^{(x)}(\tau)$ and $P_{iJ}^{(x)}(\tau)$ of the 3×3 matrices $\hat{\mathbf{Q}}^{(x)}(\tau)$ and

$\hat{\mathbf{P}}^{(x)}(\tau)$. Consequently, it is sufficient to solve only 12 DRT equations instead of 18 DRT equations.

(3) There is no need for the two point ray tracing. Only an orthonomic system of rays starting from the point source S, which intersect the target surface Σ^{tar}, should be computed.

(4) Eq. (28) is applicable to models with structural interfaces, with which the wavefield interacts on the way from the point source to the target surface Σ^{tar}. It is only necessary to take into account the transformation relations for ray tracing and DRT at interfaces and consider the complete energy reflection/transmission coefficients when evaluating amplitudes.

(5) Eq. (28) is applicable to the computation of elementary Green function related to any direct, reflected/transmitted, multiply reflected, converted elementary wave propagating in an inhomogeneous anisotropic or isotropic medium.

(6) The target surface Σ^{tar} used in the computation may be chosen in different ways. It may be chosen as a convenient geometrical surface, but it may also be taken along the Earth's surface or any structural interface. It may differ for each receiver and for each elementary Green function. It is, however, also possible to compute the complete wave field, consisting of several elementary Green functions and recorded at several receivers, using the same target surface Σ^{tar}. For the receivers distributed in a volume, one should preferably use integral superposition of Gaussian packets.

(7) The receiver R, at which we wish to use eq. (28) to evaluate the wavefield, may be situated either at an arbitrary point of the target surface Σ^{tar} or close to it. It can be situated at any point of the medium, including ray-theory shadow regions.

(8) The elementary Green function as an integral superposition of Gaussian beams (28) represents a basis for computing the high-frequency wavefield generated by various types of point sources, for example, explosive, single-force or moment-tensor point sources.

When using the Gaussian beam integral superposition of elementary Green function, one must take into account that the quality of the superposition in the singular regions of the ray method depends on the choice of the 2×2 matrix $\mathbf{M}$ of Gaussian beam parameters.

We concentrated on elementary Green functions related to elementary seismic body waves propagating independently (without mutual coupling) in laterally inhomogeneous anisotropic media. In the forthcoming paper, we plan to extend the described procedure to laterally inhomogeneous weakly anisotropic media. In such media, the two S waves may propagate coupled to large distances from sources, and require a special treatment, see, for example, Pšenčík, Farra & Tessmer (2012). Such a treatment removes shear-wave singularities, in addition to the removal of caustics problems described in this paper. P waves in such media are described by significantly simpler formulae. In parallel, we are planning a paper with numerical examples of the use of the presented formulae in some specific situations.

Let us emphasize that the formulae presented in this paper are rather general. They simplify considerably if simpler models and configurations are considered. One example is smooth laterally inhomogeneous media without structural interfaces used in most of the previous studies. In this case, the reflection/transmission coefficients in eq. (28) vanish, and with them also vanish their possible singularities. There are many other specific situations, in which the use of the integral superposition of Gaussian beams will prove to be useful.

ACKNOWLEDGEMENTS

We would like to express our gratitude to Luděk Klimeš for his stimulating comments. We are also grateful to Jean Virieux, AE of the GJI and two anonymous referees for their useful comments. We thank the Research Project 16-05237S of the Grant Agency of the Czech Republic and the project 'Seismic waves in complex 3-D structures' (SW3D) for support.

REFERENCES

Aki, K. & Richards, P.G., 1980. *Quantitative Seismology: Theory and Methods*, W.H. Freeman.

Alkhalifah, T., 1995. Gaussian beam depth migration for anisotropic media, *Geophysics,* **60,** 1474–1484.

Babich, V.M. & Popov, M.M., 1981. Propagation of concentrated acoustical beams in three-dimensional inhomogeneous media (in Russian), *Akust. Zh.,* **27,** 828–835.

Bakker, P.M., 1998. Phase shift at caustics along rays in anisotropic media *Geophys. J. Int.,* **134,** 515–518.

Bleistein, N., 2007. *Mathematical Modeling, Migration and Inversion with Gaussian Beams*. Lecture Notes, Center for Wave Phenomena, Colorado School of Mines, 118 pp.

Bleistein, N. & Gray, S.H., 2010. Amplitude calculations for 3-D Gaussian beam migration using complex-valued traveltimes, *Inverse Probl.,* **26,** 085017, 1–36.

Burridge, R., 1976, *Some Mathematical Topics in Seismology,* Courant Institute of Mathematical Sciences, New York University.

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

Červený, V., 1985. Gaussian beam synthetic seismograms, *J. Geophys.,* **58,** 44–72.

Červený, V., 2001. *Seismic Ray Theory,* Cambridge Univ. Press.

Červený, V. & Klimeš, L., 2010. Transformation relations for second order derivatives of travel time in anisotropic media, *Stud. Geophys. Geod.,* **54,** 257–267.

Červený, V. & Pšenčík, I., 1983. Gaussian beams and paraxial ray approximation in three-dimensional elastic inhomogeneous media, *J. Geophys.,* **53,** 1–15.

Červený, V. & Pšenčík, I., 2010. Gaussian beams in inhomogeneous anisotropic layered structures, *Geophys. J. Int.,* **180,** 798–812.

Červený, V., Popov, M.M. & Pšenčík, I., 1982. Computation of wave fields in inhomogeneous media. Gaussian beam approach, *Geophys. J. R. astr. Soc.,* **88,** 43–79.

Červený, V., Klimeš, L. & Pšenčík, I., 2007. Seismic ray method: recent developments, *Adv. Geophys.,* **48,** 1–126.

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

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

Gajewski, D. & Pšenčík, I., 1990. Vertical seismic profile synthetics by dynamic ray tracing in laterally varying layered anisotropic structures, *J. geophys. Res.,* **95,** 11 301–11 315.

Gao, Z., Sun, J., Sun, H., Sun, X., Yu, P. & Liu, M., 2017. A fast algorithm for prestack Gaussian beam migration adopting the steepest descent approximation, *Stud. Geophys. Geod.,* **61,** 576–587.

Garmany, J., 2001. Phase shifts at caustics in anisotropic media, in *Anisotropy 2000: Fractures, Converted Waves and Case Studies,* pp. 419–425, eds Ikelle, L. & Gangi, A., Soc. Explor. Geophysicists.

George, T., Virieux, J. & Madariaga, R., 1987. Seismic wave synthesis by Gaussian beam summation: a comparison with finite differences, *Geophysics,* **52,** 1065–1073.

Gray, S., 2005. Gaussian beam migration of common shot records, *Geophysics,* **70,** S71–S77.

Gray, S.H. & Bleistein, N., 2009. True-amplitude Gaussian-beam migration, *Geophysics,* **74,** S11–S23.
Hanyga, A., 1986. Gaussian beams in anisotropic elastic media, *Geophys. J. R. astr. Soc.,* **85,** 473–503.
Hill, N.R., 1990. Gaussian beam migration, *Geophysics,* **55,** 1416–1428.
Hill, N.R., 2001. Prestack Gaussian beam depth migration, *Geophysics,* **66,** 1240–1250.
Kendall, J.-M., Guest, W.S. & Thomson, C.J., 1992. Ray theory Green's function reciprocity and ray-centered coordinates in anisotropic media, *Geophys. J. Int.,* **108,** 364–371.
Klimeš, L., 1984. Expansion of high-frequency time harmonic wavefield given on an initial surface into Gaussian beams, *Geophys. J. R. astr. Soc.,* **79,** 105–118.
Klimeš, L., 1989. Optimization of the shape of Gaussian beams of a fixed length, *Stud. Geophys. Geod.,* **33,** 146–163.
Klimeš, L., 1994. Transformations for dynamic ray tracing in anisotropic media, *Wave Motion,* **20,** 261–272.
Klimeš, L., 2010. Phase shift of the Green function due to caustics in anisotropic media, *Stud. Geophys. Geod.,* **54,** 268–289.
Klimeš, L., 2012. Zero-order ray-theory Green tensor in a heterogeneous anisotropic elastic medium, *Stud. Geophys. Geod.,* **56,** 373–382.
Klimeš, L., 2014a. Superposition of Gaussian packets in heterogeneous anisotropic media, in *Seismic Waves in Complex 3-D Structures,* **24,** 127–130, online at http://sw3d.cz.
Klimeš, L., 2014b. Phase shift of a general wavefield due to caustics in anisotropic media, in *Seismic Waves in Complex 3-D Structures,* **24,** 95–109, online at http://sw3d.cz.
Klimeš, L., 2016. Superposition of Gaussian beams and column Gaussian packets in heterogeneous anisotropic media, in *Seismic Waves in Complex 3-D Structures,* **26,** 123–130, online at http: sw3d.cz.
Kravtsov, Yu.A. & Berczynski, P., 2007. Gaussian beams in inhomogeneous media: a review, *Stud. Geophys. Geod.,* **51,** 1–36.
Leung, S., Qian, J. & Burridge, R., 2007. Eulerian Gaussian beams for high-frequency wave propagation, *Geophysics,* **72,** SM61–SM76.
Nowack, R.L. & Aki, K., 1984. The two-dimensional Gaussian beam synthetic method: Testing and application, *J. geophys. Res.,* **89,** 7797–7819.
Popov, M.M., 1982. A new method of computation of wave fields using Gaussian beams, *Wave Motion,* **4,** 85–97.
Popov, M.M., Semtchenok, N.H., Popov, P.M. & Verdel, A.R., 2010. Depth migration by the Gaussian beam summation method, *Geophysics,* **75,** S81–S93.
Protasov, M.I., 2015. 2-D Gaussian beam imaging of multicomponent seismic data in anisotropic media, *Geophys. J. Int.,* **203,** 2021–2031.
Protasov, M.I. & Tcheverda, V.A., 2012. True amplitude elastic Gaussian beam imaging of multicomponent walkaway vertical seismic profiling data, *Geophys. Prospect.,* **60,** 1030–1042.
Pšenčík, I. & Teles, T.N., 1996. Point source radiation in inhomogeneous anisotropic structures, *Pure appl. Geophys.,* **148,** 591–623.
Pšenčík, I. & Farra, V., 2014. First-order *P*-wave ray synthetic seismograms in inhomogeneous, weakly anisotropic, layered media, *Geophys. J. Int.,* **198,** 298–307.
Pšenčík, I., Farra, V. & Tessmer, E., 2012. Comparison of the FORT approximation of the coupling ray theory with the Fourier pseudospectral method, *Stud. Geophys. Geod.,* **56,** 35–64.
Ralston, J., 1983. Gaussian beams and the propagation of singularities, in *Studies in Partial Differential Equations,* vol. 23, pp. 206–248, ed. Littman, W., Math. Ass. of Am. Studies in Mathematics.
Vinje, V., Roberts, G. & Taylor, R., 2008. Controlled beam migration: a versatile structure imaging tool, *First Break,* **26,** 109–113.
Virieux, J. & Farra, V., 1991. Ray tracing in 3-D complex isotropic media: an analysis of the problem, *Geophysics,* **56,** 2057–2069.
Weber, M., 1988. Computation of body-wave seismograms in absorbing 2-D media using the Gaussian beam method: comparison with exact methods, *Geophys. J.,* **92,** 9–24.
White, B., Norris, A., Bayliss, A. & Burridge, R., 1987. Some remarks on the Gaussian beam summation method, *Geophys. J. R. astr. Soc.,* **89,** 579–636.
Zhu, T., Gray, S.H. & Wang, D., 2007. Prestack Gaussian-beam depth migration in anisotropic media, *Geophysics,* **72,** S133–S138.

APPENDIX A: RAY TRACING IN INHOMOGENEOUS ANISOTROPIC MEDIA

Let us introduce the 3×3 *generalized Christoffel matrix* $\hat{\mathbf{\Gamma}}(x_m, p_n)$ with Cartesian components Γ_{ik}, given by the relation:

$$\Gamma_{ik} = a_{ijkl} p_j p_l = \rho^{-1} c_{ijkl} p_j p_l \,. \tag{A1}$$

Here $c_{ijkl} = c_{ijkl}(x_n)$ are real-valued elastic moduli (components of the fourth-order stiffness tensor), $\rho(x_m)$ is the density. The symbol a_{ijkl} denotes the density-normalized elastic moduli, $a_{ijkl} = c_{ijkl}/\rho$. The quantities $p_i = \partial T/\partial x_i$ are the components of the slowness vector, where $T(x_n)$ is the traveltime. The generalized Christoffel matrix is symmetric and positive definite. It has three positive eigenvalues $G(x_i, p_j)$, which are in this paper considered to be mutually different, and three corresponding eigenvectors $\mathbf{g}(x_i, p_j)$. They correspond to the three elementary waves, P, S1 and S2, propagating in inhomogeneous anisotropic media. The eigenvalues $G(x_i, p_j)$ and the eigenvectors $\mathbf{g}(x_i, p_j)$ are the solutions of the Christoffel equation

$$(\Gamma_{ik} - G\delta_{ik})g_k = 0 \tag{A2}$$

and of its characteristic equation (condition of solvability of (A2)):

$$\det(\Gamma_{ik} - G\delta_{ik}) = 0. \tag{A3}$$

The eigenvalues $G(x_i, p_j)$ of the generalized Christoffel matrix $\hat{\mathbf{\Gamma}}$ represent basic elements in the *eikonal equations* $G(x_i, p_j) = 1$ controlling kinematics of each of the three elementary P, S1 or S2 waves. In the *Hamiltonian form*, the eikonal equation reads:

$$\mathcal{H}(x_i, p_j) = \frac{1}{2} G(x_i, p_j) = \frac{1}{2}. \tag{A4}$$

The eikonal eq. (A4) is a nonlinear partial differential equation of the first order for the traveltime $T = T(x_i)$. It can be solved in terms of characteristics. The equations of characteristics, *ray-tracing equations*, have the form:

$$\frac{\mathrm{d}x_i}{\mathrm{d}u} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \frac{\mathrm{d}p_i}{\mathrm{d}u} = -\frac{\partial \mathcal{H}}{\partial x_i}, \quad \frac{\mathrm{d}T}{\mathrm{d}u} = p_i \frac{\partial \mathcal{H}}{\partial p_i} \,. \tag{A5}$$

Here u is a monotonic parameter along the characteristics (ray). The choice of the *Hamiltonian function* $\mathcal{H}(x_i, p_j)$ in the form (A4), that is, as a homogeneous function of the second degree in p_i, and the use of the Euler's theorem lead to

$$p_i \frac{\partial \mathcal{H}}{\partial p_i} = 2\mathcal{H} = 1. \tag{A6}$$

As a consequence of (A6), the third equation in (A5) yields $\mathrm{d}T/\mathrm{d}u = 1$, that is, the parameter u along the ray is traveltime. We denote this parameter τ. We emphasize that τ represents the traveltime T only along the ray Ω, not in its vicinity.

A1 Ray tracing system

As shown above, it is not necessary to calculate T along the ray by solving the last equation in (A5). The traveltime $T = \tau$ is automatically obtained by solving the ray-tracing system, which consists of six nonlinear ordinary differential equations of the first order:

$$\frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \frac{\mathrm{d}p_i}{\mathrm{d}\tau} = -\frac{\partial \mathcal{H}}{\partial x_i}. \tag{A7}$$

The partial derivatives of the Hamiltonian in (A7) can be expressed in several alternative forms. The most straightforward is

$$\frac{\partial \mathcal{H}}{\partial p_i} = \mathcal{U}_i = a_{ijkl} p_l g_j g_k, \quad -\frac{\partial \mathcal{H}}{\partial x_i} = \eta_i = -\frac{1}{2} \frac{\partial a_{jkln}}{\partial x_i} p_k p_n g_j g_l. \tag{A8}$$

The symbols $\mathcal{U}_i$ and η_i denote Cartesian components of the ray-velocity vector $\boldsymbol{\mathcal{U}}$ and the vector $\boldsymbol{\eta}$, the derivative of the slowness vector $\mathbf{p}$ with respect to the traveltime τ.

A2 Point-source initial conditions for rays

To solve the ray-tracing system (A7), the initial values $\mathbf{x}(\tau_0)$, $\mathbf{p}(\tau_0)$ for the initial traveltime$\tau = \tau_0$ must be specified. We denote the initial point with coordinates $\mathbf{x}(\tau_0)$ by S, that is, $\mathbf{x}(S) = \mathbf{x}(\tau_0)$. It remains to specify $\mathbf{p}(S)$. It is common to specify $\mathbf{p}(S)$ by the ray parameters γ_1, γ_2, that is, by parameters determining one specific ray. At the point S, the ray parameters γ_1, γ_2 are usually taken as the take-off angles φ_0, δ_0. The initial conditions for $p_i(S)$ then read:

$$p_i(S) = \mathcal{C}^{-1}(S; \mathbf{N}(S)) N_i(S) \,. \tag{A9}$$

Here $\mathbf{N}(S)$ is a unit vector at the point S specified by take-off angles φ_0 and δ_0 in the following way:

$$\mathbf{N}(S) \equiv (\cos\varphi_0 \cos\delta_0,\ \sin\varphi_0 \cos\delta_0,\ \sin\delta_0) \,. \tag{A10}$$

The symbol $\mathcal{C}(S; \mathbf{N}(S))$ denotes the phase velocity corresponding to the direction $\mathbf{N}(S)$,

$$\mathcal{C}(S; \mathbf{N}(S)) = [G(x_i(S), N_j(S))]^{1/2} \,, \tag{A11}$$

where $G(x_i, N_j)$ is one of the three eigenvalues of the generalized Christoffel matrix $\hat{\mathbf{\Gamma}}(x_i, p_j)$ defined in (A1), with p_j replaced by N_j. Eq. (A11) follows from the fact that $G(x_i, p_j)$ is a homogeneous function of the second degree in p_j, and $G(x_i, p_j) = 1$, see eq. (A4). Therefore, $G(x_i, p_j) = \mathcal{C}^{-2}(x_i, N_j) G(x_i, N_j) = 1$, which yields (A11). It is important to emphasize that the take-off angles φ_0, δ_0 do not specify the initial direction of the ray, but the direction of the slowness vector $\mathbf{p}(S)$ corresponding to the initial direction of the ray. The initial direction of the ray is given by the ray-velocity vector $\boldsymbol{\mathcal{U}}(S)$. The ray-velocity vector $\boldsymbol{\mathcal{U}}(S)$ may be simply calculated from $\mathbf{p}(S)$ using the first set of equations in (A8). Determination of $\mathbf{p}(S)$ from $\boldsymbol{\mathcal{U}}(S)$ is, however, a more complicated task, for which no exact explicit formulae exist. Usually, $\mathbf{p}(S)$ is determined from $\boldsymbol{\mathcal{U}}(S)$ by a procedure used in the two-point ray tracing.

For the extension of the above ray-tracing equations to layered anisotropic media, see, for example, Gajewski & Pšenčík (1987) or Červený (2001, section 2.3.3).

APPENDIX B: DYNAMIC RAY TRACING IN INHOMOGENEOUS ANISOTROPIC MEDIA

DRT consists in the solution of a system of linear ordinary differential equations of the first order along the ray Ω. The DRT system in Cartesian coordinates was studied by several authors. For a detailed derivations and for references see Červený (2001; chap. 4).

B1 Reduced DRT system in Cartesian coordinates x_i

The reduced DRT in Cartesian coordinates consists of 12 linear ordinary differential equations for $Q_{iK}^{(x)} = \partial x_i / \partial \gamma_K$ and $P_{iK}^{(x)} = \partial p_i / \partial \gamma_K$, where γ_K are ray parameters. The DRT system reads:

$$\begin{aligned} \mathrm{d}Q_{iK}^{(x)}/\mathrm{d}\tau &= A_{ij}^{(x)} Q_{jK}^{(x)} + B_{ij}^{(x)} P_{jK}^{(x)}, \\ \mathrm{d}P_{iK}^{(x)}/\mathrm{d}\tau &= -C_{ij}^{(x)} Q_{jK}^{(x)} - D_{ij}^{(x)} P_{jK}^{(x)}, \end{aligned} \tag{B1}$$

where

$$\begin{aligned} A_{ij}^{(x)} &= \partial^2 \mathcal{H} / \partial p_i \partial x_j \,, \quad B_{ij}^{(x)} = \partial^2 \mathcal{H} / \partial p_i \partial p_j \,, \\ C_{ij}^{(x)} &= \partial^2 \mathcal{H} / \partial x_i \partial x_j \,, \quad D_{ij}^{(x)} = \partial^2 \mathcal{H} / \partial x_i \partial p_j \,, \end{aligned} \tag{B2}$$

and where the Hamiltonian $\mathcal{H}(x_i, p_j)$ is given by (A4). The elements of 3×3 matrices $A_{ij}^{(x)}$, $B_{ij}^{(x)}$, $C_{ij}^{(x)}$ and $D_{ij}^{(x)}$ satisfy three symmetry relations:

$$B_{ij}^{(x)} = B_{ji}^{(x)} \,, \quad C_{ij}^{(x)} = C_{ji}^{(x)} \,, \quad D_{ij}^{(x)} = A_{ji}^{(x)} \,. \tag{B3}$$

The elements $Q_{iK}^{(x)}$ and $P_{iK}^{(x)}$ of 3×3 matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ in (B1) are required to satisfy the following constraint relation:

$$\mathcal{U}_i P_{iK}^{(x)} - \eta_i Q_{iK}^{(x)} = 0 \tag{B4}$$

along the ray Ω. The symbols $\mathcal{U}_i$ and η_i denote components of the ray-velocity vector $\boldsymbol{\mathcal{U}}$ and eta vector $\boldsymbol{\eta}$, respectively.

B2 Point-source initial conditions for the DRT

Let us consider the ray parameters γ_1 and γ_2 to be the take-off angles $\gamma_1 = \varphi_0$ and $\gamma_2 = \delta_0$, for which the unit vector $\mathbf{N}(S)$, specifying the direction of the slowness vector at the point S, has the form (A10).

The initial conditions for $Q_{iJ}^{(x)}$ are straightforward:

$$Q_{iJ}^{(x)}(S) = 0 \,. \tag{B5}$$

For the determination of the initial conditions for $P_{iJ}^{(x)}$, we have to differentiate the slowness vector at the point S with respect to γ_1 and γ_2. We get

$$P_{iJ}^{(x)}(S) = [Z_{iJ}(S) - p_i(S) \mathcal{U}_k(S) Z_{kJ}(S)] / \mathcal{C}(S; \mathbf{N}(S)), \tag{B6}$$

where $Z_{iJ}(S) = \partial N_i(S) / \partial \gamma_J$. For Z_{iJ} we get:

$$\begin{aligned} &Z_{11}(S) = -\sin\varphi_0 \cos\delta_0, \quad Z_{21}(S) = \cos\varphi_0 \cos\delta_0, \\ &Z_{31}(S) = 0, \\ &Z_{12}(S) = -\cos\varphi_0 \sin\delta_0, \quad Z_{22}(S) = -\sin\varphi_0 \sin\delta_0, \\ &Z_{32}(S) = \cos\delta_0. \end{aligned} \tag{B7}$$

See Pšenčík & Teles (1996, eq. A4) for the derivation and more details.

With the initial conditions (B5) and (B6), the elements $Q_{iK}^{(x)}$ and $P_{iK}^{(x)}$ of 3×3 paraxial matrices $\hat{\mathbf{Q}}^{(x)}$ and $\hat{\mathbf{P}}^{(x)}$ along the ray Ω have the meaning of partial derivatives of spatial coordinates and of components of the slowness vectors with respect to γ_K.

For the extension of the reduced DRT to layered anisotropic media, see, for example, Farra & LeBégat (1995) or Pšenčík & Farra (2014).