Diffraction and seismic tomography

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SUMMARY

Diffraction tomography is formulated in such a way that the data (traveltime—or waveform perturbations) are related to the medium perturbations through the sum of two terms. The first term is the ray integral of ordinary tomography and involves only phase perturbations. The additional diffraction term involves both phase and amplitude perturbations. The diffraction term is linear in the gradients of the velocity perturbation in an acoustic medium, the gradients of the elastic and density perturbations in an elastic medium, and the gradients of the boundary perturbations across the wave is crossing. This formulation has the additional advantage that unwanted diffractions from the non-physical boundary of the region under study can be easily removed. Acoustic scattering, elastic scattering, and scattering by boundary perturbations are analyzed separately. Attention is paid to the adequacy of the acoustic approximation, and to the difference between perturbations of a boundary level (topography) and perturbations of boundary conditions. These differences are irrelevant for ordinary seismic tomography. All results are based on first-order approximations (Born or Rytov), as is the case for other published methods of diffraction tomography.

Key words: boundary perturbation, diffraction tomography, scattering theory, seismic tomography.

INTRODUCTION

Tomographic methods have played an increasingly important role in many fields where ray theory is applicable to describe the propagation of waves. Very efficient inversion algorithms have been developed for situations where sources and receivers are placed at regular intervals in a homogeneous background medium, as is common in X-ray medical applications (Barrett 1984). Similar algorithms have been used in seismic cross-well tomography (see e.g. Worthington 1984, and references therein). However in seismological applications, sources and receivers are usually located at irregular intervals, and the homogeneous background medium is often not a good assumption. To some extent the same may be true for cross-well tomography. Thus seismic tomography usually cannot take direct advantage of fast transform methods. However the problem of traveltime inversion can be posed in the form of a general linearized inverse problem, and in this form seismic tomography has been widely applied both for exploration purposes (Worthington 1984; Ivansson 1987), in lithospheric studies (Aki, Christoffersson & Husebye 1977) and to study the Earth's deep interior (Dziewonski, Hager & O'Connell 1977).

Despite the widespread application of these methods, a number of limitations were recognized at an early stage. A fundamental limitation is due to the neglect of wave diffraction off the geometrical ray path. This neglect limits the resolution of tomographic results in general. The limitation is especially serious in circumstances where diffraction effects dominate the observations, as may be expected in the presence of low-velocity regions among others (Wielandt 1987). To overcome these limitations, diffraction effects have been taken into account, in a first-order approximation, in methods called diffraction tomography (e.g. Devaney 1984). It was later recognized that these methods, when applied to reflection data, are closely connected to wavefront migration (Miller, Oristaglio & Beylkin 1987). However in accord with the original formulation of tomography, current methods in diffraction tomography assume a homogeneous background medium and regular sampling of the wavefield, such that Fourier transform methods can be used for the solution of the scattering problem at hand. In its present form these methods are of limited use, at least in earthquake seismology.
In this paper, diffraction tomography will be formulated in such a way that the observation variable (a traveltime residual, or more general a waveform perturbation) is approximated by the sum of a geometrical ray term which itself is the basis of ordinary seismic tomography, and a diffraction term which is an integral over the volume of heterogeneity and over the surface of boundary perturbations. The integrand is linear in the gradients of heterogeneity perturbations (velocity, elastic constants, and density) and the gradients of the boundary perturbations sampled by the wavefield. This means that diffraction tomography can still be posed in the form of a linearized inverse problem. The results are based on first-order scattering theory as in the case for other published methods of diffraction tomography. In the following we separately consider acoustic and elastic scattering, and scattering by boundary perturbations.

### Acoustic Scattering

Consider the wave motion \( u(x, t) \) in a medium with velocity \( c \), slowness \( s = 1/c \) and density \( \rho \). The reference medium has velocity \( c^0 \), slowness \( s^0 = 1/c^0 \), and the wave motion is \( u^0(x, t) \). The slowness perturbation in a volume \( V \) is \( \delta s = s - s^0 \), and the ensuing scattered wave motion is \( \delta u = u - u^0 \). No density perturbations are assumed here; acoustic scattering with density variations has been treated by Stolt & Weglein (1985); perturbations in both the density and in the elastic parameters are treated in the next section, on elastic scattering. A standard procedure using the Born approximation gives (e.g. Aki & Richards 1980)

\[
\delta u(x, t) = - \int_V 2pc \delta s \mathbf{G} \cdot \mathbf{u}^0 \, dV
\]

where \( \mathbf{G} \) is the Green's tensor for the medium. Let \( \mathbf{u}^0 \) and \( \mathbf{G} \) be given by ray theory:

\[
\mathbf{u}^0(\xi, t) = \mathbf{v}^0(\xi)A^0(\xi)f(t - T^0),
\]

\[
\mathbf{G}(x, \xi, t) = \mathbf{v}(x)\mathbf{v}^T(\xi)A^1(x, \xi) \delta(t - T^1).
\]

Quantities associated with the incident and scattered wave have superscripts 0 and 1, respectively; \( \mathbf{v} \), \( \mathbf{v}^0 \), \( \mathbf{v}^1 \) are unit displacement vectors, and \( A^0 \), \( A^1 \) are amplitude factors. \( A^0 \) and \( A^1 \) are allowed to be complex, but this requires a generalization of equations (2) and (3) such that for example \( A^0 f(t) \) is replaced by \( \Re(A^0 f(t) - \mathcal{H}_A^0 f(t)) \), where \( g(t) \) is the Hilbert transform of \( f(t) \). We assume this generalization in all the following equations if required, although for simplicity we have not brought this out in the notation. Substitution in equation (1) gives

\[
\delta u(x, t) = - \int_V 2pcA^0 A^1 \mathbf{v}(x)(\mathbf{v}^0 \cdot \mathbf{v}^1) \delta s \bar{f}(t - T^0 - T^1) \, dV
\]

which is a well-established result (cf. Coates & Chapman 1990).

Each component of \( \delta u \) can be written in the form

\[
\delta u_i(x, t) = - \int_V W(\mathbf{v}^0 \cdot \mathbf{v}^1) \delta s \bar{f}(t - \tau) \, dV
\]

where

\[
\tau = T^0 + T^1
\]

and

\[
W = 2pcA^0 A^1 \mathbf{v}(x).
\]

Equation (5) is transformed into

\[
\delta u_i(x, t) = - \int_{S_{\tau}} \bar{f}(t - \tau) \int_{S_{\tau}} W(\mathbf{v}^0 \cdot \mathbf{v}^1) \delta s J dS_{\tau} \, d\tau
\]

where \( S_{\tau} \) is the surface \( \tau = \text{constant} \), and \( J \) is the Jacobian of the transformation (see Fig. 1). The transformation to an integration over what is called isochron surfaces \( S_{\tau} \) has been applied before (e.g. Haddon & Buchen 1981; Miller et al. 1987; Cao & Kennett 1989). The lower integration limit in the \( \tau \) integral is the stationary traveltime of the geometric ray, and we have chosen the upper limit such that the bounding surface of \( V \) coincides with \( S_{\tau_0} \) for constant \( \tau_0 \). In the notation it is implicit that we have assumed the stationary traveltime \( \tau_0 \) to be a minimum with respect to path variations due to scattering points in \( V \). If \( \tau_0 \) is a maximum with respect to these variations we have to reverse the integration limits, and for a 'minimax' time (i.e. \( \tau_0 \) is a saddle point with respect to the relevant path variations) the integral is to be split, but the final results will be essentially
Fire 1. Schematic diagram showing the ray between 0 (source) and 1 (receiver), with stationary traveltime \( \tau_m \). Also shown is a section of isochron surface \( S_r \), and the surface normal to the ray is \( S_s \). Surface \( S_r \) is defined by all points \( \xi \) such that the total traveltime of the two rays connecting \( (\xi, 0) \) and \( (\xi, 1) \) is \( \tau \).

the same. Integration by parts gives

\[
\delta u_\sigma(x, t) = -\int_{S_m} W(v^0 \cdot v^1) \delta s \, J_m \, dS_m + \int_{S_u} W(v^0 \cdot v^1) \delta s \, J_u \, dS_u - \int V W(v^0 \cdot v^1) \frac{\partial}{\partial \tau} f(t - \tau) \, dV
\]

where we have neglected the variation of \( W \), since it is coupled to \( \delta s \) and would produce a second-order effect. (However, variations in \( W \) would have to be retained in a similar integral equation for \( u^0 \).) The integration surface \( S_m \) in equation (8) encloses the infinitesimal volume \( \delta V_m \) about the geometric ray. Let the ray path be parametrized by \( \sigma \), with limits \( \sigma_0 \) and \( \sigma_1 \). Then

\[
\delta V_m = \int_{\sigma_0}^{\sigma_1} \delta S_m(\sigma) \, d\sigma
\]

where \( \delta S_m \) is an infinitesimal element of surface normal to the ray in \( \sigma \) (see Fig. 1). Within this surface we can expand the time (Farra & Madariaga 1987):

\[
\tau = \tau_m + \frac{1}{2} \delta q^T C \delta q
\]

where \( \delta q \) denotes the position (in ray centred coordinates) within \( \delta S_m \), and

\[
C = Q_0^{1-1} - Q_1^{-1-1}.
\]

The \( 2 \times 2 \) matrices

\[
Q^0 = \left( \frac{\partial q(\sigma)}{\partial p(\sigma_0)} \right), \quad Q^1 = \left( \frac{\partial q(\sigma)}{\partial p(\sigma_1)} \right)
\]

define the geometrical spreading between \( \sigma_0 \) and \( \sigma \) and between \( \sigma_1 \) and \( \sigma \), respectively (Červený 1985). Here \( p(\sigma) \) is the 2-D slowness vector, in ray centred coordinates. For minimum traveltime \( \tau_m \), the quadratic form in equation (9) is positive for all \( \delta q \), and

\[
\delta q^T C \delta q = a = \text{constant}
\]

is the equation of an ellipse with area \( \pi a / |C|^{1/2} \). Hence the surface area \( \delta S_m \) bounded by \( \tau = \text{constant} \) can be obtained by putting \( a = 2(\tau - \tau_m) = 2 \delta \tau \):

\[
\delta S_m(\sigma) = 2\pi \delta \tau \, |C|^{1/2}.
\]

Using this result in equation (8), we have

\[
J_m \, dS_m = \frac{2\pi}{|C|^{1/2}} \, d\sigma.
\]

Moreover, following Coates & Chapman (1990):

\[
\frac{1}{|C|^{1/2}} = \frac{|Q_0^{1/2}| |Q_1^{1/2}|}{|Q|^{1/2}}
\]

where

\[
Q = \left( \frac{\partial q(\sigma_1)}{\partial p(\sigma_0)} \right)
\]
is the spreading matrix between $a_0$ and $a_1$. The amplitude factor of the incident wave (equation 2) is

$$A^0 = \pm (\rho c |Q|)^{-1/2} \tag{13}$$

where the $\pm$ sign corresponds to the minimum/maximum time character of the ray between $a_0$ and $a_1$; for a minimax ray, $|Q^0|$ is negative and $A^0$ will be imaginary. The result (13) needs to be generalized if multiple caustics exist. These can be taken into account by introducing the so-called KMAH index $\sigma$ (Chapman 1985; Coates & Chapman 1990) and replacing $A^0$ by $|A^1| \exp(i\sigma/2)$. The index $\sigma$ increases by an integer (normally 1) each time the ray touches a caustic surface.

The amplitude factor of the Green's function (equation 3) is

$$A^1 = \pm \frac{1}{4\pi} (\rho c_1 |Q|)^{-1/2} \tag{14}$$

The rules for the sign, and the required generalization if multiple caustics exist, are the same as for $A^0$.

Combining equations (6) and (11)–(14) we can rewrite the first term of equation (8):

$$\delta u_i^m(x, t) = \mp \int_{S_m} W(v^0 \cdot v^1) \delta s J_m dS_m = -\delta u_i^m(x, t) \int_{S_0} \delta s d\sigma \tag{15}$$

where

$$\delta u_i^m(x, t) = v_i(x) A(x) f(t - \tau_m) \tag{16}$$

and

$$A(x) = \pm (\rho c_1 |Q|)^{-1/2}$$

To proceed with the other terms of equation (8), we attach to each point $\xi$ in $V$ a unit vector $\eta$ normal to the surface $\tau = \text{constant}$ in the direction of increasing $\tau$. For $\xi$ not close to the geometric ray,

$$\eta = (p^0 - p^1)/|p^0 - p^1| \tag{17}$$

and

$$d\tau/d\eta = |p^0 - p^1| \tag{18}$$

where $p^0$ and $p^1$ are the 3-D slowness vectors of the incident and scattered waves, respectively. In the second term of equation (8) we then have

$$J_m = (d_\tau |d\eta|)^{-1} = |p^0 - p^1|^{-1} \tag{19}$$

In the third term of equation (8),

$$\frac{\partial \delta s}{\partial \tau} = \eta \cdot \nabla \delta s / d\eta = (p^0 - p^1) \cdot \nabla |p^0 - p^1|^2 \tag{20}$$

Although this result is not valid close to the ray, it is obvious from symmetry considerations that, provided $\delta s$ is continuous in any small surface area $\delta S_m$ normal to the ray in $\sigma$ and bounded by $\delta \tau = \text{constant}$:

$$\int_{\delta S_m} \frac{\partial \delta s}{\partial \tau} d\tau = 0,$$

hence, $\nabla \delta s$ does not contribute in a region bounded by $\delta \tau = \text{constant}$ close to the ray, and this region can be excluded from integration.

Summarizing, using equation (15), (19) and (20) we rewrite equation (8):

$$\delta u_i(x, t) = -\delta u_i^m(x, t) \int_{S_0} \delta s d\sigma f(t - \tau_m) \int_{S_m} W(v^0 \cdot v^1) \frac{\delta s}{|p^0 - p^1|^2} dS_m - \int_{V} W(v^0 \cdot v^1) \frac{(p^0 - p^1) \cdot \nabla \delta s}{|p^0 - p^1|^2} f(t - \tau) dV. \tag{21}$$

This first term is just the first term of a Taylor series expansion of $u_i(x, t)$ due to a change in geometrical traveltine. Coates & Chapman (1990) obtained the equivalent phase delay term in the frequency domain, by a different method. The second term expresses diffraction from the boundary of $V$. If the boundary is non-physical, this term should be deleted (the implicit assumption being $\delta s = \text{constant outside} V$). The third term expresses diffraction due to changes in the velocity perturbation.
\[ \nabla \delta s. \text{ Retaining the first and the third term, } \delta u_i^m \text{ and } \delta u_i^n, \text{ we have in the frequency domain} \]
\[ \delta U_i(x, \omega) = \delta U_i^m(x, \omega) + \delta U_i^n(x, \omega) = i\omega U_i^m(x, \omega) \int_{V} \delta s \, d\sigma + i\omega F(\omega) \int_{V} W(\psi^0 \cdot \nu^1) \frac{(p^0 - p^1) \cdot \nabla \delta s}{|p^0 - p^1|^2} \exp(i\omega \tau) \, dV. \] (22)

The Rytov approximation is (Tarantola 1987, p. 484)

\[ \ln \frac{U_i(x, \omega)}{U_i^m(x, \omega)} = i\omega \int_{V} \delta s \, d\sigma + \frac{1}{\nu(x)A(x)} \int_{V} W(\psi^0 \cdot \nu^1) \frac{(p^0 - p^1) \cdot \nabla \delta s}{|p^0 - p^1|^3} \exp[i\omega(\tau - \tau^m)] \, dV. \] (23)

The first term in the brackets is the usual ray integral of seismic tomography. The second term is the basis of diffraction tomography. The integration volume \( V \) can be chosen so as to include (an appropriate fraction of) the Fresnel zone. We anticipate that the degree of improvement of the tomographic image depends primarily on an accurate estimate of the phase \( \omega \tau \) in the diffraction integral. Thus \( \tau \) may have to be calculated iteratively using previous tomographic results. Preliminary results suggest that inclusion of the diffraction integral can be a significant improvement even when inverting only traveltime residuals (cf. Witten & King 1990). In the latter case only the real part of the integral is used in the inversion; the imaginary part gives the amplitude perturbation.

Any of the velocity or slowness parametrization schemes in common use will convert equation (23), (22) or (21) to a form that is linear in the slowness parameters, so that standard inverse methods can be applied. The common case of a block parametrization is special in the sense that the diffraction term contributes only diffractions from the block boundaries. Thus, at the boundary \( S_{jk} \) between two adjacent blocks \( j \) and \( k \):

\[ \nabla \delta s = -[\delta s]_k \nabla \delta S_{jk} \]

where \( \nabla \delta s \) is the surface normal pointing into block \( k \), and \( \delta S_{jk} \) is the delta-function on \( S_{jk} \). The diffraction term is then

\[ \delta u_i^j(x, t) = \sum_j \sum_{k > j} \int_{S_{jk}} W(\psi^0 \cdot \nu^1) \frac{(p^0 - p^1) \cdot \nabla \delta s}{|p^0 - p^1|^3} \delta(t - \tau) \, dS \] (24)

where the sum over \( k \) is restricted to blocks adjacent to \( j \), and the additional restriction \( k > j \) is used to avoid duplicating interfaces.

**ELASTIC SCATTERING**

The problem of first-order elastic scattering (Born approximation) has been treated by many authors (e.g. Hudson 1977). Our purpose here is to emphasize the agreements and differences between the results for the elastic and the acoustic case. In particular, we are interested in the range of validity of the acoustic scattering assumption. We assume an isotropic medium, and use \( \delta \rho, \delta \kappa \) and \( \delta \mu \) to denote the perturbations in density, incompressibility and rigidity, respectively. The first Born approximation leads to

\[ \delta u(x, t) = \int_{V} G \ast S \, dV \] (25)

with (Doornbos & Mondt 1979):

\[ S = -\delta \rho \frac{u^0}{\rho} + \left( \delta \kappa - \frac{4}{3} \delta \mu \right) \nabla (\nabla \cdot u^0) - \delta \mu \nabla \times \nabla \times u^0 + (\nabla \cdot u^0) \nabla \left( \delta \kappa - \frac{2}{3} \delta \mu \right) + 2\epsilon^0 \delta \mu \] (26)

and the strain tensor \( \epsilon^0 \) has the elements

\[ e^0_{ij} = \frac{1}{2} \left[ \delta \mu \right]_{ij} + \partial u_i^j. \]

Substituting equations (2) and (3) for the incident wave and the Green's function, we can write the scattered field in a form similar to equation (4):

\[ \delta u(x, t) = -\int_{V} v(x)A^0 A^1 \rho \sum_{a,b} \delta a \delta b \int (t - T^a - T^b) \, dV \] (27)

where

\[ g_1 = \delta \rho / \rho, \quad a_1 = (v^0 \cdot v^1), \quad g_2 = \delta \kappa / \kappa, \quad a_2 = -\left( 1 - \frac{4}{3} \epsilon \right) (v^0 \cdot v^0) (v^1 \cdot v^1), \]

\[ g_3 = \delta \mu / \mu, \quad a_3 = -\epsilon \frac{C_1}{C_0} \left[ (v^0 \cdot v^1) (v^0 \cdot v^1) + (v^0 \cdot v^1) (v^1 \cdot v^1) - \frac{2}{3} (v^0 \cdot v^0) (v^1 \cdot v^1) \right]. \] (28)
Here \( \gamma \) and \( \nu \) are unit vectors in the direction of wave propagation and displacement, respectively, \( c \) is the wave velocity (\( a \) for \( P \), \( \beta \) for \( S \)), and \( \varepsilon = \beta^2/c^2 \). Quantities associated with the incident and scattered wave have superscripts 0 and 1, respectively.

Examining equations (27) and (4) reveals that the acoustic factor

\[
V_{ac} = 2c \frac{\delta c (\nu^0 \cdot \nu^1)}{c} = -2 \frac{\delta c}{c} (\nu^0 \cdot \nu^1)
\]

is replaced, for elastic scattering, by

\[
V_{ei} = \sum_{i=1}^{3} a_i R_i.
\]

Thus we can use equations (28)–(30) to assess the validity of acoustic scattering. The velocity perturbations can be expressed, assuming \( \alpha^2/\beta^2 = 3 \):

\[
-2 \frac{\delta \alpha}{\alpha} = \frac{5 \delta \kappa}{\kappa} - 4 \frac{\delta \mu}{\mu}, \quad -2 \frac{\delta \beta}{\beta} = \frac{\delta \rho}{\rho} - \frac{\delta \mu}{\mu}.
\]

For \( P \rightarrow P \) scattering, from equation (28) and using \( \cos \phi = (\nu^0 \cdot \nu^1) \):

\[
V_{ei}(P) = \cos \varphi \frac{\delta \rho}{\rho} - \frac{5 \delta \kappa}{9 \kappa} \frac{2}{9} (3 \cos^2 \varphi - 1) \frac{\delta \mu}{\mu}.
\]

and for \( S \rightarrow S \) scattering:

\[
V_{ei}(S) = \cos \varphi \frac{\delta \rho}{\rho} - (2 \cos^2 \varphi - 1) \frac{\delta \mu}{\mu}.
\]

Thus for forward scattering in the so-called specular direction, \( \varphi = 0 \) and \( V_{ac} = V_{ei} \) in the Born approximation, for both \( P \)- and \( S \)-waves (Aki & Richards 1980). For \( \varphi \neq 0 \) the error \( (V_{ac} - V_{ei}) \) depends on the relative perturbations of \( \rho \), \( \kappa \) and \( \mu \). To get a rough estimate of this error we adopt, from Anderson (1989):

\[
\frac{\delta \beta}{\beta} = 2 \frac{\delta \alpha}{\alpha} = 1.5 \frac{\delta \rho}{\rho}
\]

hence

\[
\frac{\delta \mu}{\mu} = 4.5 \frac{\delta \kappa}{\kappa} = 1.35 \frac{\delta \rho}{\rho}.
\]

With these quantities, the relative error

\[
\varepsilon = (V_{ac} - V_{ei})/V_{ac}
\]

increases, for \( P \) from 0 for \( \varphi = 0^\circ \), to 20 per cent for \( \varphi = 27^\circ \), and to 100 per cent for \( \varphi = 60^\circ \). The relative error for \( S \) increases from 0 for \( \varphi = 0^\circ \), to 20 per cent for \( \varphi = 18^\circ \), and to 100 per cent for \( \varphi = 40^\circ \). To judge the significance of these numbers, consider a typical tomographic experiment with teleseismic data aimed to map upper mantle structure at about 100 km depth from data near 60° epicentral distance. Including half the Fresnel zone in the diffraction term gives \( \phi_{max} = 10^\circ \) for \( P \) at 1 s period, and \( \phi_{max} = 50^\circ \) at 20 s period. If 20 per cent is taken as an acceptable relative error, then the acoustic approximation is acceptable for \( P \) up to a period of about 5 s. the corresponding numbers for \( S \) are: \( \phi_{max} = 10^\circ \) at 1 s period, \( \phi_{max} = 40^\circ \) at 20 s period, and the acceptable period range for the acoustic approximation is up to about 4 s. For longer periods, diffraction tomography might proceed using a prescribed scaling relation between the relative perturbations of \( \rho \), \( \kappa \) and \( \mu \).

**A BOUNDARY PERTURBATION**

Perturbations of internal boundaries and of the Earth's surface must be treated different from relatively smooth velocity perturbations. The difference arises both in seismic tomography and in scattering theory. In tomography the traveltime perturbation of a wave being transmitted through or reflected from a boundary that is displaced over a distance \( h \), is obtained by a simple geometrical analysis of the wavefront:

\[
\delta \tau = (p^0_v - p^s_v) h.
\]

(34)

Without loss of generality we assume here and in the following that the reference level is horizontal. Then \( h \) is the vertical displacement of the boundary from the reference level, and \( p_v \) is the vertical component of the slowness vector. Superscripts 0 and 1 denote the incident and scattered waves, respectively; in what follows we will use the same notation to identify the
velocities and densities at the two sides of the boundary. Using scattering theory, we want to generalize the above result in analogy to the result (23) for velocity perturbations, such that equation (34) still gives the ray contribution in addition to the diffraction term.

In scattering theory, the generalization of reflection/transmission coefficients for a plane boundary to coefficients for a rough boundary has been given in the form of a perturbation series (Doornbos 1988). For our present purpose we need the first two terms of this series, including the Born approximation. Let the reference level be the \( z = 0 \) plane, then the boundary perturbation is characterized by \( z = h(\xi_x, \xi_y) \), where \( \xi_x, \xi_y \) are coordinates in the \( z = 0 \) plane, and the (non-unit) normal to the boundary is \( n = (-\partial h/\partial x, -\partial h/\partial y, 1)^T \). It is appropriate to determine first a displacement-traction vector at the boundary. Let \( \mathbf{u} \) be the displacement components, \( \mathbf{r} \) the associated stress tensor, and \( \sigma = r_{ik} n_k \) the modified traction components. The appropriate displacement-traction vector is, for a solid–solid interface:

\[
\mathbf{d} = (u_x, u_y, u_z, \sigma_x/\omega, \sigma_y/\omega, \sigma_z/\omega)^T.
\]

For a free surface,

\[
\mathbf{d} = (u_x^+, u_y^+, u_z^+, \sigma_x/\omega, \sigma_y/\omega, \sigma_z/\omega)^T
\]

where the superscript \( + \) denotes the field below the surface. For a solid–liquid interface,

\[
\mathbf{d} = (u_x^+, u_y^+, \mathbf{n} \cdot \mathbf{u}, \mathbf{n} \cdot \sigma/\omega)^T
\]

where \( u_x^+, u_y^+ \) are horizontal displacement components in the solid which is here assumed above the interface.

The solution for \( \mathbf{d} \) is obtained in the horizontal wavenumber domain. We define

\[
\mathbf{D}(k_i) = \int_{-\infty}^{+\infty} \mathbf{d}(\xi_x, h) \exp(-i k_i \cdot \xi_x) \, d\xi_x
\]

where \( \xi_x = (\xi_x, \xi_y)^T \) and \( k_i = (k_x, k_y)^T \). We also define an incident wave vector \( \mathbf{A}^0(k_i) \exp(ik_i \cdot \xi_x) \) containing the wavenumber components of up- and downgoing \( P, SV \) and \( SH \). The complete solution for \( \mathbf{d}(\xi_x, h) \) would require \( \mathbf{D}(k_i) \) for all wavenumbers \( k_i \). Within the present context this is not a practical solution. Instead we will approximate the solution for \( \mathbf{d} \) in such a way that it is consistent with \( \mathbf{D}(k_i) \) for the particular wavenumber \( k_i \) given by the Green’s function (equation 3) that accounts for propagation between the scatterer in \( \xi \) and the receiver in \( x \). The required approximation is

\[
\mathbf{d}(\xi_x, h) = (\mathbf{P}^0)^{-1}(k_i^0) \exp(i k_i h) \left( \mathbf{P}^0(k_i^0) + \frac{\partial h}{\partial x} \mathbf{X}^0(k_i^0) + \frac{\partial h}{\partial y} \mathbf{Y}^0(k_i^0) \right) (\mathbf{P}^0)^{-1}(k_i^0) \mathbf{A}^0(k_i^0) \exp(i k_i^0 \cdot \xi_x).
\]

Here \( \mathbf{P}^0, \mathbf{X}^0 \) and \( \mathbf{Y}^0 \) are reflectivity matrices introduced by Doornbos (1988). They play the same role as the matrices arising in the calculation of ordinary reflection/transmission coefficients. In fact, \( \mathbf{P}^0 \) is just the matrix needed for calculating the coefficients for a plane horizontal boundary. The additional matrices are needed to satisfy conditions at the sloping boundary. The diagonal matrix \( \exp(ik_i h) \) contains the vertical wavenumbers \( k_i \) for up- and downgoing \( P, SV \) and \( SH \). It acts as a propagator matrix between the reference level at \( z = 0 \) and the boundary at \( z = h \). Substituting \( \mathbf{d}(\xi_x, h) \) in equation (35), expanding \( \exp(ik_i h) \) in a Taylor series, and retaining the zeroth- and first-order terms,

\[
\mathbf{D}(k_i) = \mathbf{D}^{(0)}(k_i) + \mathbf{D}^{(1)}(k_i),
\]

it is easily verified that the resulting expressions for \( \mathbf{D}^{(0)} \) and \( \mathbf{D}^{(1)} \) are indeed equivalent to those given by Doornbos (1988).

The scattered wave coefficient vector \( \mathbf{B}(k_i) \) can be obtained by the matrix integral equation (cf. Doornbos 1988):

\[
\mathbf{B}(k_i) = \int_{-\infty}^{+\infty} \exp(i k_i h) \left( \mathbf{P}^i(k_i^0) - \frac{\partial h}{\partial x} \mathbf{X}^i(k_i^0) - \frac{\partial h}{\partial y} \mathbf{Y}^i(k_i^0) \right) \cdot \mathbf{d}(\xi_x, h) \exp(-i k_i \cdot \xi_x) \, d\xi_x,
\]

where \( \mathbf{P}^i, \mathbf{X}^i \) and \( \mathbf{Y}^i \) are reflectivity matrices in analogy to the ones introduced in equation (36). We assume now that there is just one type of incident wave \( \mathbf{A}_{inc}^0 \), such that in equation (36) we do not need the complete inverse matrix \( (\mathbf{P}^0)^{-1}(k_i^0) \), but only the appropriate column \( (\mathbf{P}^0)^{-1}(k_i^0) \). Likewise we consider one type of scattered wave \( \mathbf{B}_{sc} \), and we need in equation (37) only the appropriate row vectors \( \mathbf{P}_{sc}^T, \mathbf{X}_{sc}^T \) and \( \mathbf{Y}_{sc}^T \), and the appropriate vertical wavenumber \( k^i \). We note that for any of the up- and downgoing waves, the vertical wavenumber \( K = \pm \omega p_z \) where \( p_z \) is the vertical component of the slowness vector. In the following we use \( K = \omega Z \) and \( K^i = -\omega p_z^i \) (this follows from the sign conventions used in Doornbos 1988). Combining equations (36) and (37) with the above specifications, and expanding \( \exp(i \omega Z h) \) and \( \exp(-i \omega p_z^i h) \) in Taylor series, we get the following result up to order one:

\[
\mathbf{B}_{sc}(k_i) = \int_{-\infty}^{+\infty} [R(k_i^0, k_i^0) + i \omega h R^i(k_i^0, k_i^0) + \nabla h \cdot \mathbf{R}^{11}(k_i^0, k_i^0)] \mathbf{A}_{inc}^0(k_i^0) \exp(-i (k_i^0 - k_i) \cdot \xi_x) \, d\xi_x,
\]
The expression for the scattered field $u(x, t)$ requires a slight modification of the result (38). Firstly, the coefficient $B_{sc}(k_y)$ is associated with the plane wave component of a Weyl integral. It can be associated with the Green's tensor (3) by rewriting, in the frequency domain:

$$G(x, 5, \omega) = v(x)v''(5)\gamma'(5)\exp(i\omega T),$$

(42)

where $Q^T(k_y)$ is the appropriate factor in the Weyl integral. Secondly, the wavenumber of the incident and scattered waves, $k_p$ and $k_y$, vary with scatterer position $\xi$, on the boundary. Combining equations (38) and (42) and transforming the result to the time domain, we get

$$u_s(x, t) = \int \left[ W[R + \nabla h \cdot R']f(t - \tau - hR'f(t - \tau)]\gamma_y \right] dS$$

(43)

where $W$ is given by equation (6), and $\gamma_y$ is the vertical component of the unit wave direction vector, i.e. $p_x = \gamma_y/c$. The term with $R$ produces the zeroth-order field. The perturbation is due to the terms with $R'$ and $R''$. There may be an additional perturbation due to rapid lateral changes of $R$; we consider this possibility in the next section, but ignore the perturbation here. Thus

$$\delta u_s(x, t) = -\int \left[ WhR'hJ_y \gamma_y dS \right]$$

(44)

The term with $h$ can be treated in the same way as equation (5). Thus we transform the integral

$$-\int WhR'hJ_y \gamma_y dS = -\int \gamma_y \int WR'hJ_y d\tau d\tau$$

(45)

where $\gamma_y$ is the trajectory $\tau = constant$ (i.e. an isochron, see Fig. 2). Repeating the steps leading to equation (8), we get here

$$-\int f(t - \tau_m) \int WR'hJ_y \gamma_y d\tau d\tau$$

(46)

Note that in the first integral, $R'$ is to be evaluated for $k_y = k_y$. From equations (39) and (40):

$$R'(k_y, k_y) = (p - p_j)R(k_y, k_y)$$

(47)

To evaluate the first integral of expression (46), we use the result (10) for an infinitesimal element of surface normal to the scattered ray. The factor $\gamma_y$ is needed for the transformation to an element of surface on the reference plane. Thus (cf. equation 11)

$$\int J_y \gamma_y d\tau = \frac{2\pi}{|\mathbf{c}|^{1/2}}$$

(48)

Noting that the spreading matrix $Q^o$ in equation (12) applies to the incident wave, we have to multiply $|Q^o|$ by the factor $\gamma_y/\gamma_y$.

Figure 2. Schematic diagram showing the reflected ray between 0 (source) and 1 (receiver), with stationary traveltime $\tau_m$. Also shown is the isochron $l_\gamma$ on the reflecting surface $S$, and the surface normal to the reflected ray is $S_m$. A similar diagram applies to a refracted ray.
upon transmission through the boundary (Červený 1985). The amplitude factor \( A \) in equation (16) is similarly modified by the factor \( R(\rho^0c^0/v^0, \rho^1c^1/v^1)^{1/2} \).

Thus using equation (48), (12), (13), (14) and (16), and substituting (47),

\[
\Delta u^m_i(x, t) = -\hat{f}(t - \tau_m) \int \nabla h \cdot \mathbf{r}_m \, dl_m = \left( \rho^0 c^0 - \rho^1 c^1 \right) h \hat{u}^m_i(x, t).
\]  

(49)

It is argued, as in the previous section, that the second term of expression (46) represents diffraction from the boundary of surface \( S \), and this effect should be deleted in practical circumstances (the implicit assumption being \( h = \text{constant} \) outside \( S \)). To evaluate the last integral of (46), we repeat the development summarized by equations (17)–(20), except that we use 2-D instead of 3-D vectors, i.e. we express our results in terms of horizontal slowness vectors \( p^0_i \) and \( p^1_i \), where \( \omega p^0_i = k^0_i \) and \( \omega p^1_i = k^1_i \):

\[
\frac{\partial h}{\partial t} = (p^0_i - p^1_i) \cdot \nabla h / |p^0_i - p^1_i|^2
\]  

(50)

and an area bounded by \( \delta \tau = \text{constant} \) close to the ray can be excluded from integration.

Summarizing the results expressed by (45), (46) and (50), we can rewrite equation (44):

\[
\Delta u^m_i(x, t) = \Delta u^m_i(x, t) + \Delta u^m_i(x, t) = -\left( p^0_i - p^1_i \right) h \hat{u}^m_i(x, t) - \int_S \nabla h \cdot \left( \frac{(p^0_i - p^1_i)}{|p^0_i - p^1_i|^2} \mathbf{R}^{11} \right) \hat{f}(t - \tau) \gamma^1_i dS.
\]  

(51)

In the frequency domain:

\[
\Delta U^m_i(x, \omega) = \Delta U^m_i(x, \omega) + \Delta U^m_i(x, \omega) = i\omega (p^0_i - p^1_i) h U^m_i(x, \omega) + i\omega \int_S \nabla h \cdot \left( \frac{(p^0_i - p^1_i)}{|p^0_i - p^1_i|^2} \mathbf{R}^{11} \right) \exp(i\omega(\tau - \tau_m)) \gamma^1_i dS.
\]  

(52)

The Rytov approximation is

\[
\ln \frac{U_i(x, \omega)}{U_i^m(x, \omega)} = i\omega \left[ (p^0_i - p^1_i) h + \frac{1}{v_i(x) A(x)} \int_S \nabla h \cdot \left( \frac{(p^0_i - p^1_i)}{|p^0_i - p^1_i|^2} \mathbf{R}^{11} \right) \exp \left[ i\omega(\tau - \tau_m) \right] \gamma^1_i dS \right].
\]  

(53)

Note the similarity between equations (51–53), and equations (21)–(23) for acoustic scattering. The first term in these equations is the usual delay time of seismic tomography. However, the diffraction integral for a boundary perturbation contains an additional term \( \nabla h \cdot \mathbf{R}^{11} \) that has no counterpart in acoustic scattering. This term is needed to satisfy conditions at a non-horizontal boundary. Examination of \( \mathbf{R}^{11} \) and \( \mathbf{R}^{11} \) (equations 40 and 41) suggests that the two diffraction terms can be of comparable magnitude.

All of the remarks regarding the implementation of acoustic diffraction tomography following equation (23) are also relevant to boundary tomography following equation (53). Thus the integration surface \( S \) can be chosen to correspond to (an appropriate fraction of) the Fresnel zone, and the time \( \tau \) may have to be calculated iteratively using previous tomographic results for \( h \). The calculation of \( \mathbf{R}^{11} \) and \( \mathbf{R}^{11} \) in equation (53) is more elaborate than the calculation of the corresponding factor \( (\mathbf{v}^0 \cdot \mathbf{v}^1) \) for acoustic scattering. On the other hand, \( \mathbf{R}^{11} \) and \( \mathbf{R}^{11} \) are frequency independent, and the integration in equation (53) is 2-D rather than the 3-D diffraction integral in equation (23).

**PERTURBATION OF BOUNDARY CONDITIONS**

We reconsider the first term of the scattered field, in equation (43). The integral with the factor \( R \) can be evaluated in the same way as the integral with \( R^1 \), using equations (45)–(50). This leads to

\[
\int_S W \hat{f}(t - \tau) \gamma^1_i dS = u^m_i(x, t) + \Delta u^m_i(x, t)
\]  

(54)

and

\[
\Delta u^m_i(x, t) = \int_S \left( \frac{p^0_i - p^1_i}{|p^0_i - p^1_i|^2} \right) \nabla h \cdot \hat{f}(t - \tau) \gamma^1_i dS.
\]  

(55)

In the frequency domain:

\[
\Delta U^m_i(x, \omega) = F(\omega) \int_S \left( \frac{p^0_i - p^1_i}{|p^0_i - p^1_i|^2} \right) \nabla \exp(i\omega(\tau - \tau_m)) \gamma^1_i dS.
\]  

(56)
Diffraction and seismic tomography

In order to assess the significance of $\delta U_p^i$ due to $\nabla R$, relative to $\delta U_p^i$ due to $\nabla h$ in equation (52), we write

$$\nabla R = \frac{\partial R}{\partial \rho} \delta \rho^+ + \frac{\partial R}{\partial \rho^-} \delta \rho^- + \frac{\partial R}{\partial \kappa^+} \delta \kappa^+ + \frac{\partial R}{\partial \kappa^-} \delta \kappa^- + \frac{\partial R}{\partial \mu^+} \delta \mu^+ + \frac{\partial R}{\partial \mu^-} \delta \mu^-.$$

(57)

Hence perturbations $\delta \rho$, $\delta \kappa$, $\delta \mu$ along the boundary produce variations $\delta R$ of the order

$$\frac{\delta \rho}{\rho}, \frac{\delta \kappa}{\kappa}, \frac{\delta \mu}{\mu}.$$

On the other hand, a comparable variation due to a perturbation $\delta h$ can be deduced from equation (52), and is of the order

$$\omega (p_c^0 - p_s^0) \delta h.$$

Consider for example a bottomside reflection (PKKP) at the core–mantle boundary. A typical ray parameter value might be $2.5 \, \text{s/d}$. Take $p_c^1 = -p_s^0$. Then

$$\omega (p_c^0 - p_s^0) \delta h = 1.5 \delta h \quad \text{at} \quad 1 \, \text{Hz}.$$

Thus relative perturbations $\delta \rho/\rho$, $\delta \kappa/\kappa$, $\delta \mu/\mu$ of the order of 10 per cent would be needed to simulate the effect of a boundary perturbation $\delta h$ of the order of 100 m. This order of magnitude argument suggests that in the above situation, the effect of a boundary perturbation $\delta h$ dominates that of moderate perturbations of the elastic constants and density along the boundary. However the diffraction term due to $h$ and $\delta h$ decreases with increasing wave period and incident angle; hence in practice the relative importance of $\delta R$ and $\delta h$ would have to be assessed for the actual situation at hand.

CONCLUSIONS

Diffraction tomography can be formulated in such a way that it makes explicit the phase delay perturbation from ray theory which is the basis of ordinary seismic tomography. The phase delay term depends on the velocity perturbations along the ray in both acoustic and elastic media, and when the ray crosses a boundary an additional phase delay is induced that is proportional to the boundary level perturbation.

The additional diffraction term involves both phase and amplitude perturbations. The diffraction depends on the gradients of the velocity perturbation in an acoustic medium, the gradients of the elastic and density perturbations in an elastic medium, and the gradients of the boundary perturbations the wave is crossing. The diffraction term arises also in circumstances when the primary wave is cut off from the receiver, for example in a shadow zone. The formulae for the diffraction term due to acoustic, elastic and boundary perturbations are very similar, but the boundary perturbation requires an additional term to satisfy conditions at a sloping boundary. In the present formulation, numerical diffraction from the non-physical boundary of the region under study appears as a separate term and can thus be easily removed. This is consistent with the assumption of constant perturbations outside this region, in contrast to the conventional formulation which implies that the perturbation drops to zero outside the region under study. This aspect is especially important when inverting traveltimes, or relatively short waveform sections.

The difference between an elastic and an acoustic medium is immaterial in ordinary seismic tomography since only velocity perturbations can be retrieved. In diffraction tomography, the difference may be neglected when short-period data are used. In a realistic geometry that is representative of tomography for upper mantle structure, the acceptable period range was found to be about 5 s for $P$ and about 4 s for $S$, if half the Fresnel zone is included and the acceptable relative error is 20 per cent. For longer periods a preferred alternative would be to invert for scaled perturbations of the elastic constants and density.

Diffraction from a boundary can be induced not only by gradients of the boundary level, but also by lateral gradients of the elastic constants and densities along the boundary. The relative importance of such perturbations of boundary conditions depends on the wave period and incidence angle. A rough order of magnitude calculation suggests that in some recent tomographic studies of the core–mantle boundary, the effect of boundary level perturbations is probably more important than the effect of up to moderate perturbations of the elastic constants and densities. However one might have to reassess this conclusion in other circumstances.

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