Solid Earth

The imprint of crustal density heterogeneities on regional seismic wave propagation

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Abstract. Density heterogeneities are the source of mass transport in the Earth. However, the 3-D density structure remains poorly constrained because travel times of seismic waves are only weakly sensitive to density. Inspired by recent developments in seismic waveform tomography, we investigate whether the visibility of 3-D density heterogeneities may be improved by inverting not only travel times of specific seismic phases but complete seismograms.

As a first step in this direction, we perform numerical experiments to estimate the effect of 3-D crustal density heterogeneities on regional seismic wave propagation. While a finite number of numerical experiments may not capture the full range of possible scenarios, our results still indicate that realistic crustal density variations may lead to travel-time shifts of up to ~ 1 s and amplitude variations of several tens of percent over propagation distances of ~ 1000 km. Both amplitude and travel-time variations increase with increasing epicentral distance and increasing medium complexity, i.e. decreasing correlation length of the heterogeneities. They are practically negligible when the correlation length of the heterogeneities is much larger than the wavelength. However, when the correlation length approaches the wavelength, density-induced waveform perturbations become prominent. Recent regional-scale full-waveform inversions that resolve structure at the scale of a wavelength already reach this regime.

Our numerical experiments suggest that waveform perturbations induced by realistic crustal density variations can be observed in high-quality regional seismic data. While density-induced travel-time differences will often be small, amplitude variations exceeding $\pm 10\%$ are comparable to those induced by 3-D velocity structure and attenuation. While these results certainly encourage more research on the development of 3-D density tomography, they also suggest that current full-waveform inversions that use amplitude information may be biased due to the neglect of 3-D variations in density.

1 Introduction

Lateral variations in density are the driving force behind mass transport in the Earth, from crust to core (e.g. Kennett and Bunge, 2008; Turcotte and Schubert, 2014). They are the source of mantle convection, including the ascent of superplumes and the subduction of lithospheric plates. Knowledge of density is essential to discriminate between compositional and thermal heterogeneities (e.g. Trampert et al., 2004; Mosca et al., 2012), infer the nature of continental lithosphere (e.g. Jordan, 1975, 1978) or understand the relation between mantle convection and surface tectonics (e.g. Bunge et al., 2003; Liu and Gurnis, 2008; Warners-Ruckstuhl et al., 2012). Despite its outstanding importance for the solid-Earth sciences, the 3-D density structure of our planet remains poorly constrained.

1.1 The (in)sensitivity of seismic data to 3-D density variations

Unlike seismic velocities that can be inferred from the travel times of elastic waves, unambiguous information on density is difficult to find in most seismic observables.

Within the framework of seismic ray theory (e.g. Cerveny, 2001), seismic travel times are particularly insensitive

to density variations. In finite-frequency theory, the sensitivity of body waves to density is non-zero, but mostly confined to the immediate vicinity of sources and receivers (e.g. Tromp et al., 2005; Fichtner, 2010). The physical origin of this nearly complete absence of sensitivity lies in the scattering characteristics of density heterogeneities. When a body wave reaches a density perturbation, the resulting scattered wave propagates backwards, meaning that it cannot interfere with the incident wave unless the heterogeneity is located within one wavelength from either source or receiver (Wu and Aki, 1985; Tarantola, 1986; Trampert and Fichtner, 2013). This is in contrast to the scattered wave caused by a velocity heterogeneity, which propagates along with the incident wave, thereby leading to a finite-frequency travel-time shift (e.g. Tong et al., 1998; Marquering et al., 1999; Dahlen et al., 2000). Since scattered waves caused by density heterogeneities must exist, one may conclude that seismograms in general are sensitive to density variations, but this information cannot be contained in direct body wave travel times.

Unlike body wave travel times, the frequency-dependent travel times of Rayleigh waves reveal significant non-zero sensitivity to density variations (e.g. Takeuchi and Saito, 1972; Aki and Richards, 2002). The origin of this sensitivity can be understood intuitively with the mode-ray duality. Rayleigh waves can be seen as constructively interfering P-SV waves that reflect multiple times off the free surface. The reflection coefficient depends on density in the vicinity of the surface, thereby affecting the dispersion properties of the interference pattern. Unfortunately, Rayleigh wave sensitivity to density is strongly oscillatory, which leads to cancellation effects that leave little effective sensitivity to larger-scale variations.

At the long-period end of the seismic spectrum, the gravest normal modes of the Earth are sensitive to long-wavelength density structure as a result of the gravitational restoring force (Woodhouse, 1988; Dahlen and Tromp, 1998; Woodhouse and Deuss, 2007). This may be used to constrain density variations in the lower mantle where a low-degree structure is known to be dominant (e.g. Dziewoński et al., 1977; Becker and Boschi, 2002).

1.2 Previous work and possible future directions

Despite these difficulties, various attempts have been made to constrain 3-D density structure in the Earth. On the global scale, geodynamic data, including estimates of plate motion history and the location of subducting slabs, may be used to constrain the broad distribution of density in the mantle (Richards and Lithgow-Bertelloni, 1993; Nataf and Ricard, 1996; Simmons et al., 2010). Seismic constraints on 3-D density variations in the lower mantle were first presented by Ishii and Tromp (1999, 2001, 2004) based on long-period normal-mode measurements. The robustness of their results has, however, been questioned by various authors (e.g. Resovsky and Ritzwoller, 1999; Romanowicz, 2001; Kuo

and Romanowicz, 2002; Resovsky and Trampert, 2002). Recently, Koelemeijer et al. (2016) have shown that density estimates from previously used normal-mode data are not robust. However, with the incorporation of the latest data, these inferences can be improved significantly.

On regional scales, several authors jointly inverted body-wave travel times and gravity data under the assumption that seismic velocities and density are almost uniformly scaled to each other (e.g. Tondi et al., 2000, 2009; Maceira andAmmon, 2009). While correct for purely thermal density variations, this assumption prevents the detection of those interesting cases where velocities and density are not simply scaled due to the presence of compositional heterogeneities.

With the steadily increasing quality of seismic data, new observables with sensitivity to 3-D density variations are becoming sufficiently robust. Lin et al. (2012); Lin and Tsai (2012) propose using Rayleigh-wave ellipticity and local amplification measurements to estimate lithospheric density variations. The design of seismic observables with maximum sensitivity to density and minimum trade-offs to other parameters, e.g. velocities, has been suggested by Bernauer et al. (2014).

In addition to improving data quality, new opportunities may arise from the development of full-waveform inversion techniques that are capable of exploiting complete seismograms without being restricted to the well-known seismic phases (e.g. Chen et al., 2007; Fichtner et al., 2009; Tape et al., 2010; Fichtner et al., 2013). As shown by Rickers et al. (2012, 2013), the exploitation of scattered waves in full-waveform inversion can lead to substantial improvements in regional 3-D velocity images. However, the potential of full-waveform inversion to better constrain density variations in the crust and upper mantle remains largely unexplored.

1.3 Outline

As a first step towards full-waveform inversion for regional density structure, we present a study on the imprint of 3-D density heterogeneities in the crust on seismic wave propagation in the period range from 8 to 50 s. For this, we conduct a series of numerical experiments, where we analyse seismic wave propagation through random Earth models with variable complexity, i.e. correlation length scale. These models are designed to represent a range of plausible 3-D heterogeneous crustal environments. While wave propagation through random media has been widely used to quantify the effect of velocity heterogeneities (e.g. Frankel and Clayton, 1986; Frankel, 1989; Igel and Gudmundsson, 1997; Furumura and Kennett, 2005; Kennett and Furumura, 2008; Meschede and Romanowicz, 2015), variations in density have so far not been considered. Our experiments are intended to (i) provide rough estimates of the amplitude and travel-time variations related to realistic density variations, and (ii) better understand the physics behind density-induced waveform perturbations.
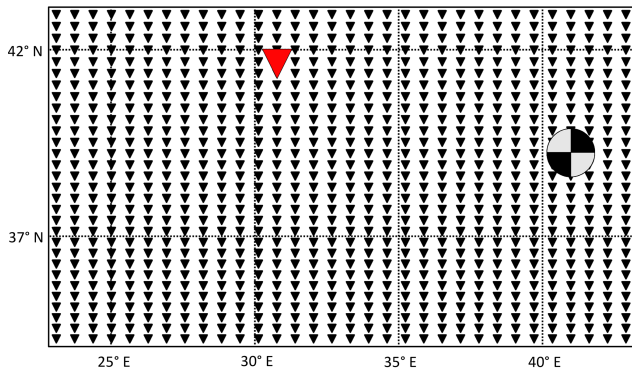
Figure 1. The grid of receivers (black triangles) on the surface of the computational domain. The source is located at 5 km depth; its location and orientation are indicated by the beach-ball plot. The receiver marked by a large red triangle and at an epicentral distance of 910 km is used for the examples presented in Sects. 3.1 and 3.2.

Following a presentation of the numerical setup, we will present detailed analyses of travel time and amplitude variations induced by 3-D crustal density heterogeneities. We expect scattering to be the dominant mechanism by which density heterogeneities influence the seismic signal. Scattering is most effective when scatterers are of similar size or smaller than the wavelength, which is why we will study the influence of frequency, propagation distance and medium complexity. Being focused on a future full-waveform inversion for density, we do not consider specific seismic phases, but try to provide ensemble estimates of waveform perturbations. Given the complexity of regional-scale seismic waveforms at periods below ∼ 20 s, it is clear that this analysis can never be complete and exhaustive. It will, however, provide a first crude estimate of the impact of crustal density structure on seismic wave propagation.

2 Setup of the numerical experiments

2.1 Numerical wave propagation

To assess the impact of 3-D density heterogeneities in the crust on seismic wave propagation, we compute numerical solutions to the elastic wave equation (e.g. Kennett, 2001; Aki and Richards, 2002)

$$\rho(\mathbf{x})\,\partial_t^2 u_i(\mathbf{x},t) - \partial_j[c_{ijkl}(\mathbf{x},t) \cdot \partial_k u_l(\mathbf{x},t)] = f_i(\mathbf{x},t),\quad (1)$$

which relates mass density ρ, the elastic tensor c_{ijkl}, and an external force f_i to the displacement field u_i. With our focus being on regional wave propagation at periods below 50 s, we can safely ignore the Earth's rotation and self-gravitation. Furthermore, we restrict ourselves to an isotropic rheology.

For the numerical solution of Eq. (1), we employ the spectral-element solver SES3-D (Fichtner et al., 2009; Gokhberg and Fichtner, 2016). The spectral-element method,

widely used in seismological research, allows us to compute accurate numerical solutions in the presence of strong 3-D heterogeneities, without requiring special treatment of the free surface (e.g. Faccioli et al., 1996; Komatitsch and Vilotte, 1998; Komatitsch and Tromp, 1999; Peter et al., 2011; Cupillard et al., 2012).

Our computational domain is a spherical section that is ∼ 2000 by ∼ 1000 km wide and 500 km deep. As a background model we use the radially symmetric preliminary reference Earth model (Dziewoński and Anderson, 1981), where we replace the original 24 km thick crust by a 40 km thick crust that better represents continental structure. Since the number of receivers has no significant impact on the computational costs of the numerical simulations, we use a dense grid of 930 receivers, distributed evenly across the surface of the computational domain. In the wave field simulations, we calculate 700 s long velocity seismograms from a strike-slip source. The complete setup is shown in Fig. 1.

2.2 Random media generation

Because the true 3-D density structure of the crust is insufficiently constrained, we use synthetic random density models in our numerical wave propagation experiments. For this, we superimpose random velocity and density variations with pre-defined correlation lengths in the horizontal and vertical directions onto the crustal part of the background model, i.e. the upper 40 km. The spatial variations in velocity and density are statistically uncorrelated, meaning that the spatial correlation averaged over many realisations is negligibly small. The individual realisations considered in this work have non-zero correlation. In Appendix Sect. A, we summarise the computation of 3-D random models based on the widely used Fourier method.

To ensure that the amplitudes of velocity and density variations are realistic, we combine information from tomographic models and empirical velocity–density scalings. For this, we compute the root-mean square (rms) of the S velocity variations in the regional crustal model of Anatolia obtained by Fichtner et al. (2013), using full-waveform inversion. S velocities at crustal depths in this model are resolved on length scales of ∼ 25 km. Using the empirical scaling relations between crustal velocities and density of Brocher (2005), we then obtain suitable ranges for variations in P velocity and density. The resulting rms variations are 260 m s^{-1} for S velocity, 460 m s^{-1} for P velocity, and 80 kg m^{-3} for density. Two particular realisations of random density variations with different correlation lengths are shown in Fig. 2. While the random models are intended to represent plausible variations of crustal structure, there exists of course uncertainty related to the poorly known amplitude spectrum of these variations in the real Earth, and the range of different velocity–density scalings proposed in the literature. We discuss these issues in more detail in Sect. 4.2. We note that random velocity and density models used in our simulations
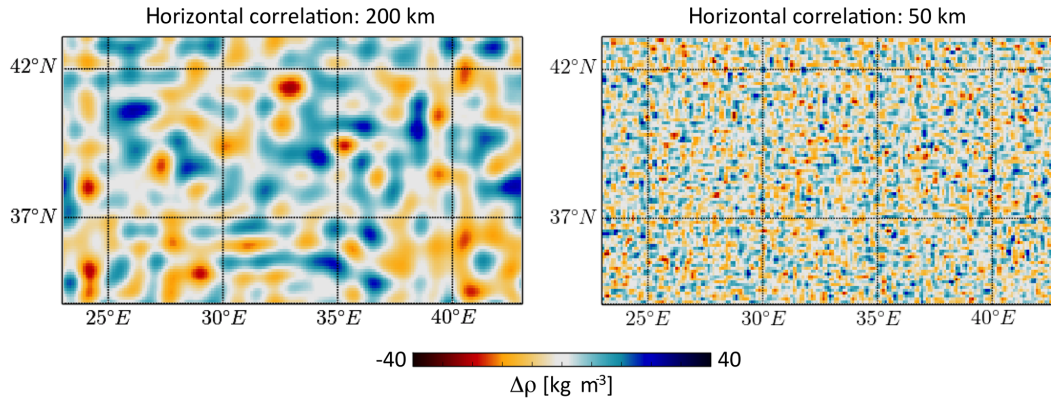
Figure 2. Realisations of random density variations. Left: 200 km lateral correlation length, 20 km vertical correlation length. Right: 50 km lateral correlation length, 10 km vertical correlation length.

are on purpose spatially uncorrelated. Empirical velocity–density scalings are used only to determine plausible rms variations.

2.3 Quantification of waveform differences

In our numerical experiments, we use media with homogeneous crustal density and random 3-D variations in P and S velocities as reference. We then compare synthetic seismograms from the reference medium with synthetic seismograms from a medium where random variations in density are added.

Since our ultimate goal is to use complete three-component seismograms to constrain density in the Earth, we do not compare isolated and well-defined seismic phases. Instead, we compute time- and frequency-dependent travel-time and amplitude differences. For this, we bandpass-filter the seismograms into a pre-defined frequency band and apply a zero-centred moving window $w(t)$ that transforms a component of a seismogram $u(t)$ into its windowed version $\hat{u}_\tau(t) = w(t - \tau)u(t)$. The travel-time difference δT as a function of τ is then defined as the argument of the maximum of the cross-correlation:

$$\delta T(\tau) = \underset{t}{\mathrm{argmax}} \int \hat{u}_\tau^{\mathrm{ref}}(t')\hat{u}_\tau(t + t')\mathrm{d}t', \qquad (2)$$

where $\hat{u}_\tau^{\mathrm{ref}}$ denotes the windowed seismogram for the reference medium with homogeneous crustal density. In the case of $\delta T < 0$, the wave for 3-D heterogeneous density arrives earlier than the reference wave, and vice versa. Similarly, we measure relative amplitude variations δA as a function of time:

$$\delta A(\tau) = \frac{\sqrt{\int [\hat{u}_\tau(t)]^2 \, \mathrm{d}t} - \sqrt{\int [\hat{u}_\tau^{\mathrm{ref}}(t)]^2 \, \mathrm{d}t}}{\sqrt{\int [\hat{u}_\tau^{\mathrm{ref}}(t)]^2 \, \mathrm{d}t}}. \qquad (3)$$

In the following sections, we consider three frequency bands of variable width: 0.02–0.125 Hz (8–50 s), 0.02–0.067 Hz

Table 1. Lateral and vertical correlation lengths of random medium variations used to assess the influence of medium complexity.

Lateral correlation length [km]	Vertical correlation length [km]
1000	100
200	20
50	10

(15–50 s), and 0.02–0.04 Hz (25–50 s). The $w(t)$ Gaussian time windows corresponding to those frequency bands have standard deviations of 8, 15 and 25 s, respectively. To stabilise the measurements, we exclude those parts of the synthetic seismograms where the average amplitude within a time window is below 5 % of the maximum within the complete trace.

While more information-rich quantifications of seismic waveform differences may be constructed, for instance on the basis of wavelet transforms (e.g. Kristekova et al., 2006, 2009), we prefer the travel time and amplitude differences defined in Eqs. (2) and (3) for their robustness and ease of interpretation. Similar quantifiers of waveform differences are frequently used in full-waveform inversion (e.g. Fichtner et al., 2008; van Leeuwen and Mulder, 2010; Bozdağ et al., 2011; Rickers et al., 2012, 2013). Since density impacts P and S energies in the same way, there is no need for any component rotation.

3 Impact of density heterogeneities on wave propagation

In the following sections, we present a phenomenological study on the impact of crustal density heterogeneities for media with different horizontal and vertical correlation lengths, summarised in Table 1. For each experiment, we compare three-component seismograms in three different
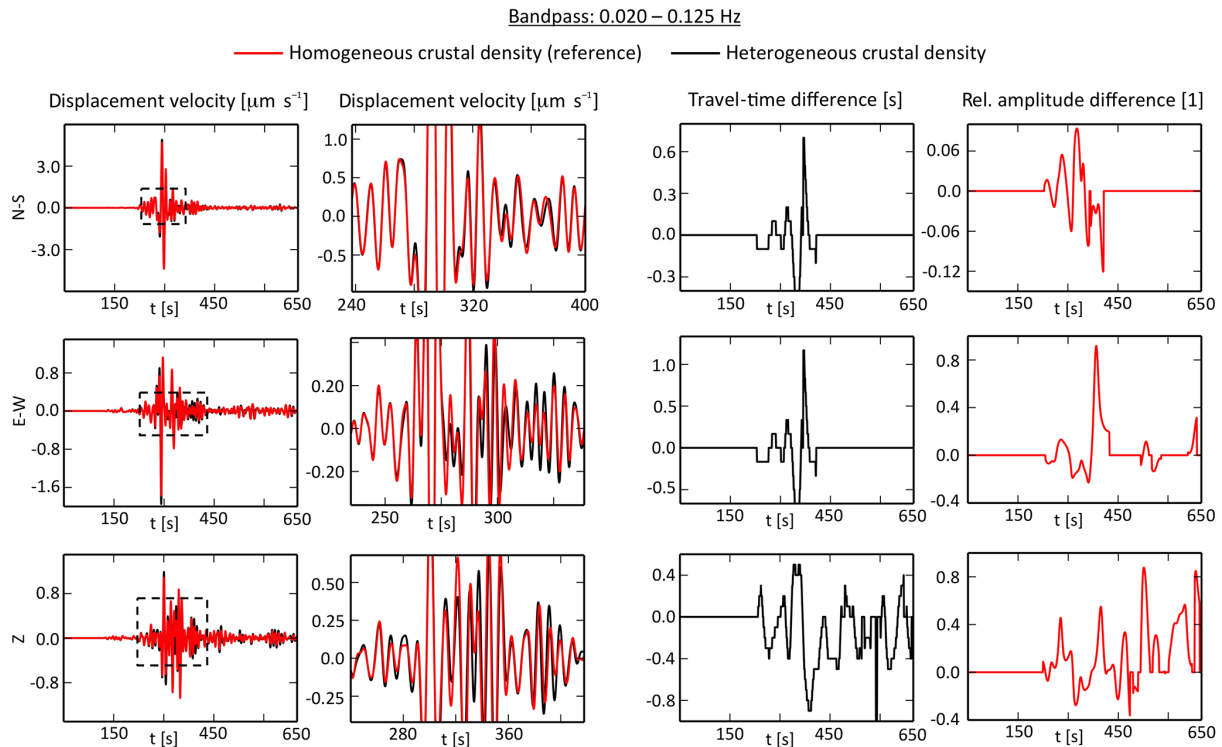
Figure 3. Comparison of synthetic seismograms for homogeneous and heterogeneous crustal densities in the broadest frequency band from 0.020 to 0.125 Hz (8–50 s). The receiver is located at an intermediate epicentral distance of 910 km, and is marked by a red triangle in Fig. 1. The correlation lengths of the heterogeneities in velocities and density are 200 km in the horizontal and 20 km in the vertical directions. The first column displays the seismograms on the N–S, E–W and Z components for the reference medium with homogeneous crustal density (red) and a medium with random heterogeneous crustal density (black). For better visibility, a zoom into the interval indicated by the black-dashed box is shown in the second column. The third and fourth columns display the time-dependent travel time and relative amplitude difference of the two sets of seismograms shown to the left. Extreme travel-time differences due to cycle skips are cropped to enhance visibility of physically meaningful travel-time variations.

frequency bands: seismograms computed for a medium with 3-D random density variations are compared with seismograms for the reference medium with homogeneous crustal density. We specifically analyse the effects of frequency (Sect. 3.2), epicentral distance (Sect. 3.3), and medium complexity (Sect. 3.4). Here and in the following sections, we use "increasing complexity" as synonymous to "decreasing correlation length".

3.1 A single-receiver example

We start with the analysis of media with 200 lateral and 20 km vertical correlation length. This will serve as a baseline for later simulations with models that have either more or less complexity. Before attempting a more comprehensive analysis in the following sections, we consider a single receiver located at 910 km epicentral distance, marked by the red triangle in Fig. 1. Figure 3 shows a comparison of three-component seismograms for homogeneous and heterogeneous crustal densities in the broadest frequency band from 0.020 to 0.125 Hz (8–50 s).

Waveform differences mostly tend to increase with increasing travel time, in accord with the expectation that (multiply) scattered waves should arrive later than the primary waves by which they have been excited. The magnitude of the time shifts are approximately independent of the component, reaching around 0.5 s. Relative amplitude differences are largest on the E–W and vertical components, where the displacement velocity itself is smallest. Therefore, low-amplitude scattered waves have the largest influence on the total amplitude. They regularly exceed 50 % in both directions, meaning that amplitudes for the heterogeneous density crust can be either twice or half as large as for the medium with homogeneous crustal density. On the N–S component, where the displacement velocity is largest, relative amplitude differences vary between ±10 %.

Figure 4 displays time shifts and relative amplitude differences for five different realisations of random media, at the same receiver and for a lower frequency band from 0.02 to 0.04 Hz. Both travel time and amplitude variations differ significantly for different media, which has two important implications: (i) different media may be distinguished from each
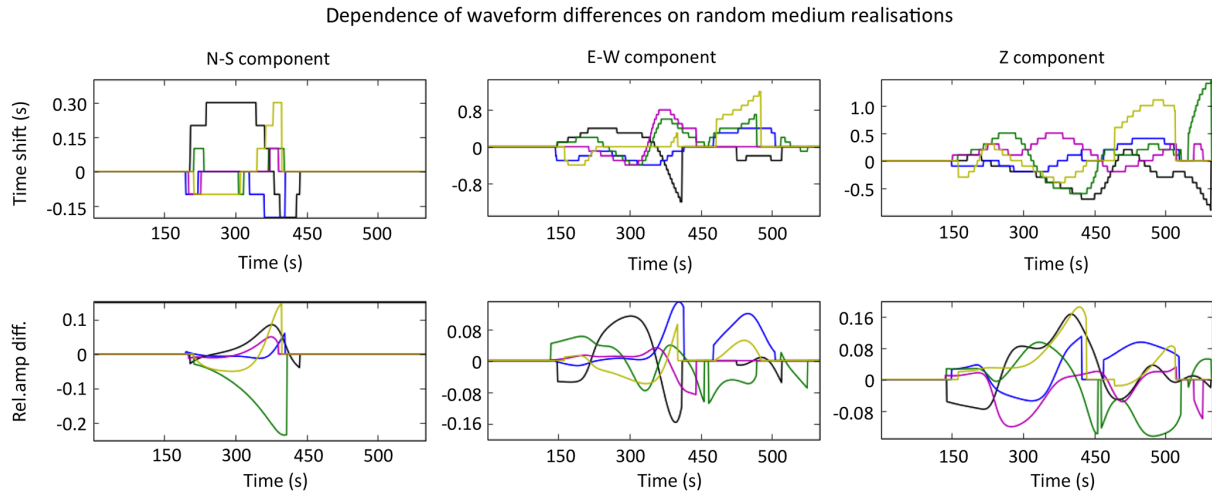
Dependence of waveform differences on random medium realisations

Figure 4. Component-wise time shifts and relative amplitude differences in the frequency band from 0.02 to 0.04 Hz for five random media realisations.

other, at least to some extent that remains to be quantified. (ii) To obtain statistically significant results in the present study, we must average travel time and amplitude variations over various random realisations. Based on our experience, five realisations are sufficient to obtain reliable results.

In addition to the dependence on the random velocity and density structure, Fig. 4 also reveals that the waveform differences in the lower frequency band from 0.02 to 0.04 Hz are on average smaller than for the higher frequency band from 0.020 to 0.125 Hz. In the following section, we will investigate this frequency dependence in more detail.

3.2 The effect of frequency

A variant of Fig. 3 for the narrower and lower frequency band from 0.02 to 0.04 Hz (25–50 s) is shown in Fig. 5. While relative amplitude differences are markedly smaller than at higher frequencies, the travel-time differences are still comparable.

This preliminary, and mostly visual, analysis of frequency dependence indicates that waveform differences are primarily caused by scattering that transfers energy from the large-amplitude N–S component onto the smaller-amplitude E–W and vertical components. Constructive and destructive interference between primary and scattered waves may cause the wave amplitudes to deviate in both directions. An increase of amplitudes may be further supported by additional wave focusing induced by 3-D density heterogeneities. The approximate frequency independence of travel-time differences, however, can hardly be explained with basic wave propagation intuition.

To make our analysis more comprehensive and efficient, we compute histograms of time shifts and relative amplitude differences for all 930 stations in the receiver grid. In line with our future goal, which is to use full-waveform inver-

sion to constrain 3-D density variations, we do not consider specific seismic phases, but longer time series that comprise body, surface and scattered waves. After calculating the misfits for all of the receivers of the grid, we stack their values into histograms, each histogram corresponding to a different frequency band. The values that we consider in the stacking procedure are measured up to 300 s after the first difference between the two waveforms (shortly after the first arrival of the P wave). This ensures, firstly, that the difference in epicentral distance between receivers does not affect the histogram shape, and secondly, that most of the waveforms with large enough amplitudes are included, while excluding low-amplitude parts of the seismograms where numerical errors have a larger impact. In order to obtain representative results, we average the measurements of time shift and relative amplitude differences over five random media realisations. Histograms showing the effect of bandwidth on time shifts and relative amplitude differences are displayed in Fig. 6.

Relative amplitude differences for the broader frequency band, i.e. for frequencies that are on average higher, have a considerably larger spread than at lower frequencies. In the 0.02–0.125 Hz band, the standard deviation of the amplitude differences is 0.15. Amplitudes can be both smaller and larger than in the reference scenario with homogeneous crustal density. Within the lower frequency band from 0.02 to 0.04 Hz, the standard deviation of the amplitude differences is reduced to 0.07, suggesting that the single-station analysis from Figs. 3 and 5 has more general validity.

The dependence of time shifts on frequency is more complex, as shown in the left panel of Fig. 6 and in Table 2. The standard deviation reaches 0.2 s for the two highest frequency bands (0.02–0.125 and 0.02–0.067 Hz), and surprisingly increases to 0.38 s for the lowermost frequency band from 0.02 to 0.04 Hz.
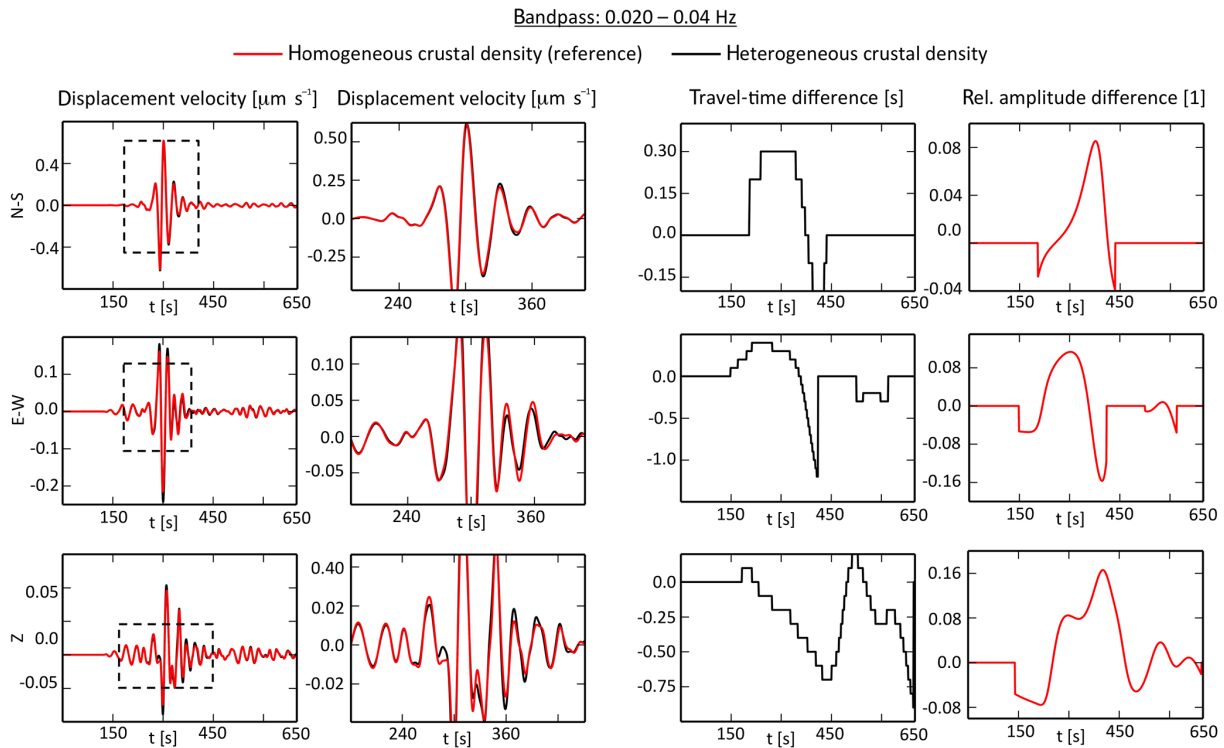
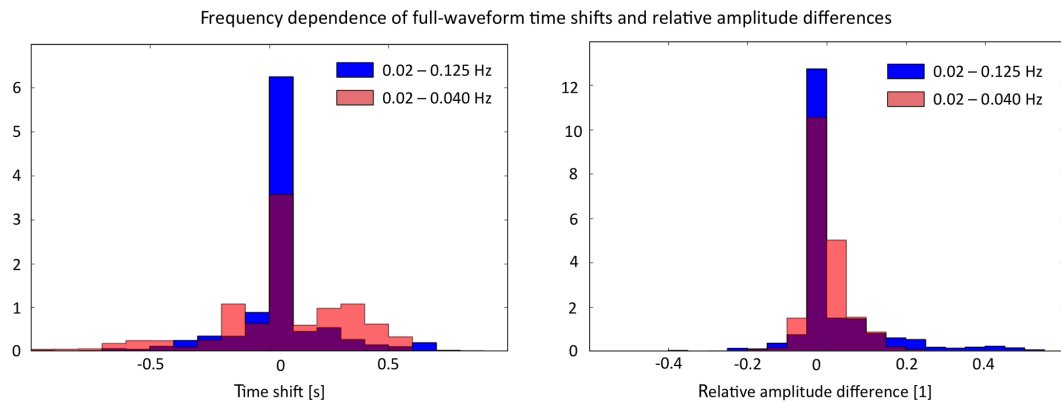**Figure 5.** The same as in Fig. 3 but for the narrowest frequency band from 0.02 to 0.04 Hz (25–50 s).

Figure 6. Normalised histograms of time shifts (left) and relative amplitude differences (right) averaged over five random media realisations with 200 km lateral and 20 km vertical correlation length. The lower frequency band from 0.02 to 0.04 Hz is shown in magenta, and the higher frequency and from 0.02 to 0.125 Hz in blue. Relative amplitude differences at higher frequencies (blue) have a visibly larger spread than at lower frequencies (magenta). The spreads of the time shift histograms are, however, comparable for both frequency bands. A summary of standard deviations in the histograms is provided in Table 2.

To investigate this phenomenon further, we show histograms for the lowest and highest frequency bands for a single random medium realisation and for the three different components in the top row of Fig. 7. We observe a distinct tail of reduced time shifts of ∼ 1 s on the E–W component and for the lowest frequency band. A similar observation can be made for two out of five random media, suggesting that these time shifts are not highly unlikely to be artefacts of

an unusual random medium realisation. The bottom row of Fig. 7 shows a pair of synthetic seismograms at an epicentral distance of ∼ 1300 km that contributes to this tail of negative time shifts – we show directly by plotting this exemplary pair that in the lower frequency band (from 0.02 to 0.04 Hz), the waveforms for the 3-D heterogeneous crust arrive early by ∼ 1 s. The tail of negative time shifts appears only for stations of distance between 1000

Frequency-dependent full-waveform time shifts for a single random medium realisation
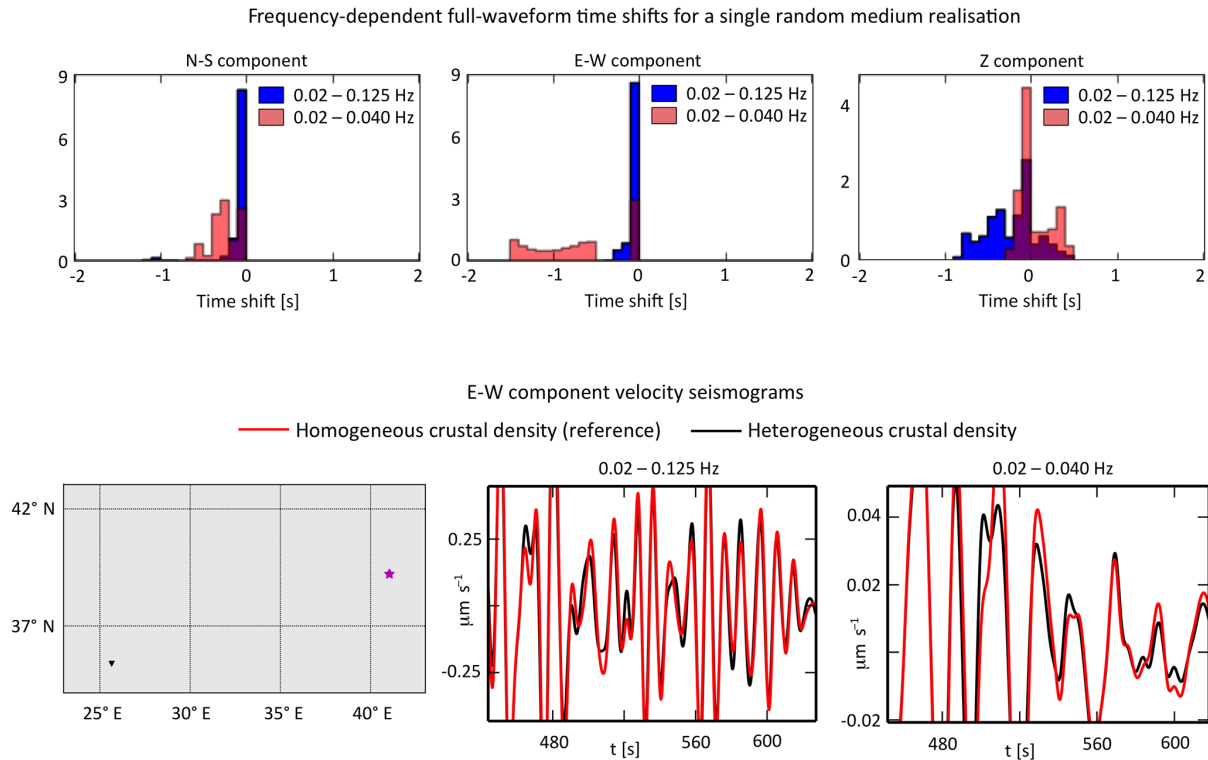

Figure 7. Top row: Normalised histograms of frequency-dependent time shifts for a single random medium realisation with 200 lateral and 20 km vertical correlation length. The lower frequency band from 0.02 to 0.04 Hz is shown in magenta, and the higher frequency and from 0.02 to 0.125 Hz in blue. The three different components are plotted separately. The isolated tail of reduced time shifts for the lowest frequency band on the E–W component was observed for two out of five random medium realisations, the average of which is shown in Fig. 6. Bottom row: Comparison of E–W component synthetic seismograms for the homogeneous reference crust (red) and the 3-D heterogeneous crust (black) for the source-receiver geometry shown in the left panel. In the lower frequency band from 0.02 to 0.04 Hz waves for the 3-D heterogeneous crust arrive early by ~ 1 s, thus contributing to the negative time shift tail in the E–W component histogram shown above. For the higher frequency band from 0.02 to 0.125 Hz, a similar effect is not visible.

and 1200 km (the far away stations) and is absent for stations of epicentral distance between 100 and 300 km (the stations close to the source). We examined this distance dependence further, using synthetic data from one of the numerical experiments contributing to the tail. For all the frequency bands for far away stations, the mean time shift value is shifted to negative values between −0.08 and −0.14 s. While the mean time-shift values are similar for all the frequencies in question, the standard deviation of time shift for the lowest frequency band is three times as big as for the other bands and reaches 0.8 s. We do not observe any of those relations for the stations close to the source. A visual waveform comparison suggests that the travel-time differences may be a finite-frequency effect, meaning that waveform (amplitude) differences within short time intervals translate into time shifts when these are measured by cross-correlation within a finite frequency band. We discuss this aspect in more detail in Sect. 4.1.

3.3 The effect of epicentral distance

To investigate whether density-related travel time and amplitude differences are only local effects or accumulate with propagation distance, we plot histograms for stations in two different epicentral distance ranges: 100–300 and 1000–1200 km. We again average over five random media realisations with 200 lateral and 20 km vertical correlation length. The results for the broadest frequency band from 0.02 to 0.125 Hz are shown in Fig. 8.

For epicentral distances between 100 and 300 km, the variance of the time shifts is 0.15 s, and it increases to 0.64 s for epicentral distances between 1000 and 1200 km. Similarly, the variance of relative amplitude differences increases from 0.007 to 0.111. This indicates that waveform differences due to crustal density heterogeneities indeed accumulate with increasing epicentral distance, which is an essential prerequisite for the use of tomographic methods.
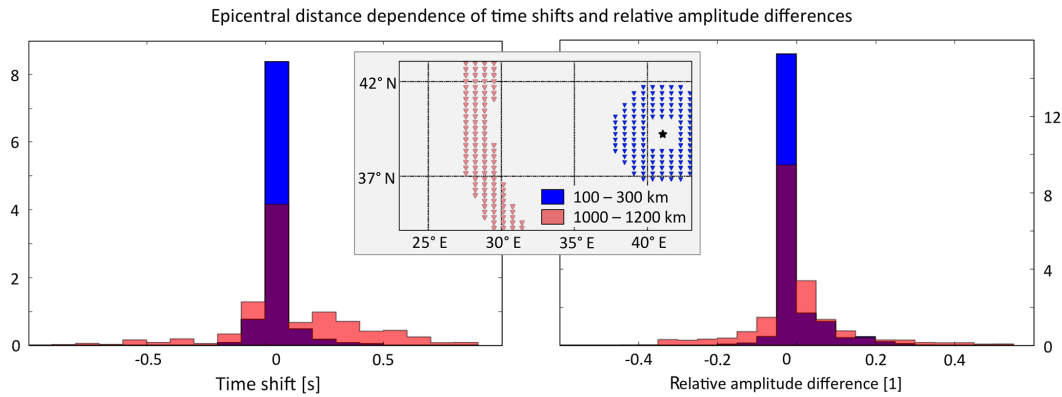
Figure 8. Normalised time shifts (left) and relative amplitude differences (right) for stations in two epicentral distance ranges: 100–300 (blue) and 1000–1200 km (magenta). The source-receiver configuration is shown in the inset. The frequency range is 0.02–0.125 Hz. The spread of both time shifts and relative amplitude differences increases with epicentral distance, indicating that the observed waveform differences accumulate with increasing propagation distance instead of being a purely local effect.

Table 2. Standard deviations of time shifts and relative amplitude differences as a function of frequency bandwidth.

Frequency band	Standard deviation of time shifts	Standard deviation of relative amplitude differences
0.02–0.04 Hz	0.38 s	0.07
0.02–0.067 Hz	0.20 s	0.06
0.02–0.125 Hz	0.19 s	0.15

3.4 The effect of medium complexity

In order to reveal the physical origin of the waveform differences, we consider random media with different lateral correlation lengths, listed in Table 1. We again work with the broadest frequency band from 0.02 to 0.125 Hz.

As shown in the top row of Fig. 9, the medium with 50 km lateral correlation length leads to a broad distribution of time shifts and relative amplitude differences, compared to the medium with 200 km lateral correlation used in the previous sections. The standard deviations of time shifts and relative amplitude differences reach values of 0.94 s and 0.20, respectively. In contrast, travel time and amplitude variations for the smooth medium, shown in the bottom row of Fig. 9, are nearly zero for all times and for all receivers. Their standard deviations are 0.01 s and 0.01, respectively.

The histograms in Fig. 9 indicate that waveform differences induced by 3-D density variations occur mostly due to scattering which is most effective when heterogeneities are equal or smaller in size than the wavelength. In a medium with 50 km lateral correlation length, the size of heterogeneities is comparable to the wavelength of waves with a maximum frequency of 0.125 Hz, and scattering becomes the dominant mechanism to perturb the wave field. In the smooth medium with 1000 km lateral correlation length, the domi-

nant mechanism is transmission, which clearly has no significant impact on either travel times or amplitudes.

4 Discussion

4.1 Seismic signatures of crustal density heterogeneities

Our numerical experiments show that 3-D crustal density heterogeneities may lead to both positive and negative variations in the travel times and amplitudes of seismic waves. This indicates that 3-D density structure leaves an imprint on regional seismic wave fields that goes beyond simple scattering attenuation of the main arrivals.

To understand the effects which play a major role in wave propagation, we look first at the misfit histograms for different frequency bands (Sect. 3.2). Intuitively, the histogram for the frequency band in which more misfits are accumulated should have smaller zero peak and bigger spread. We would expect to observe more misfits for higher frequencies due to illumination of finer structures. However, as can be seen in Fig. 6, while the peak around zero is smaller for the lower frequency band for both time shifts and amplitude differences, the spread is comparable for time shifts and larger for the higher frequency band for amplitude differences. This may mean that we observe a variety of effects that affect wave propagation and have different impact on the observed seismograms for different frequency bands. Below we discuss this seemingly counterintuitive result.

Our lowest bandwidth has a peak frequency of 0.03 Hz, which translates into a dominant wavelength of roughly 100 km for a wave travelling with the velocity of 3.2 km s^{-1} (the PREM value for crustal S velocity). Since the lateral cross-correlation length of the random medium used in our setup is 200 km, the lateral mean size of a scatterer should
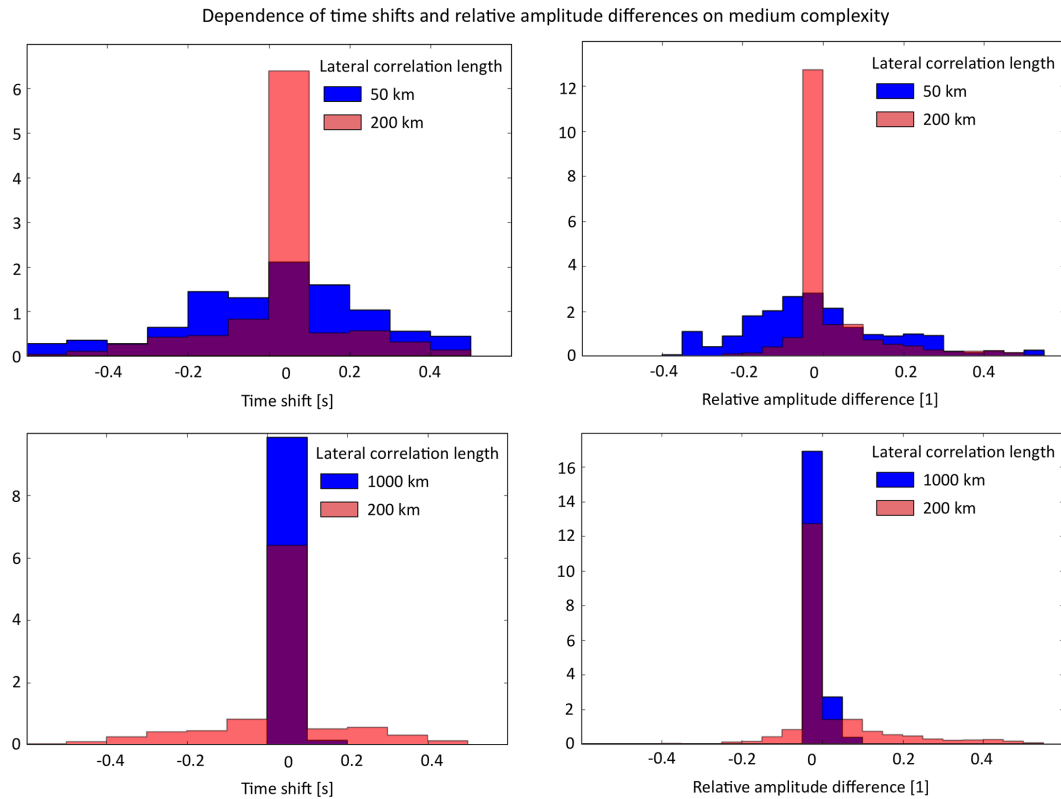
Dependence of time shifts and relative amplitude differences on medium complexity

Figure 9. Histograms of time shifts (left) and relative amplitude differences (right) for a complex medium with 50 km lateral correlation length (top, blue) and a smooth medium with 1000 km lateral correlation length (bottom, blue). The medium with 200 km lateral correlation length, used in the previous sections, is used as reference and plotted in magenta. The frequency band is 0.02–0.125 Hz. Both time shifts and relative amplitude differences grow considerably with growing complexity of the medium.

reach the value of around 100 km, which matches the dominant wavelength of the lowest bandwidth. This would mean that in this bandwidth, we will observe resonant scattering for waves travelling horizontally with the velocity of around 3.2 km s^{-1}. In consequence, due to more scattering, we will measure higher values of density-related misfits. Increasing the peak frequency to 0.07 Hz, which is the peak frequency of our highest bandwidth (0.02–0.125 Hz), would decrease the dominant wavelength for an S wave to around 50 km, and thus move us away from resonance. In that case, with increasing frequency, scattering off heterogeneities becomes less significant in favour of transmission effects. That essentially means approaching the range of the infinite-bandwidth approximation of ray theory validity, in which we completely lose sensitivity to density. Smaller scattering in higher frequencies may mean that we will observe more misfits of values around zero, causing the histograms for the higher frequency band to have larger zero peaks.

An increase of the peak frequency of the bandwidth in our particular case means observing less scattering for certain waves, however, it also means a proportional increase in relative propagation distance. This implies that we will observe waveform differences accumulated for bigger number

of wavelengths, and the amount of large non-zero density-related misfits will increase. This is an effect that changes the histogram shape in a way opposite to moving away from resonance. The larger propagation distance could then be one of the reasons behind the broader histogram spread for the higher frequency band.

Increasing the relative propagation distance is equivalent to moving further from the source, which is consistent with Sect. 3.3, where we show that density-related misfits accumulate with distance. The observation of more waveform differences with larger epicentral distance also suggests that the impact of density structure is not merely a local effect, but rather an integral over the complete wave path – an essential prerequisite for performing tomography.

While the results for different frequency bands are physically governed by the amount of scattering and the length of the relative propagation distance, and the results for different epicentral distances by the length of the propagation distance only, for various medium complexities we observe how important scattering is for sensitivity to density. The noticeable change in histogram shape in Fig. 9 is caused by much bigger amount of scattering for more complex media. The nearly complete absence of waveform differences
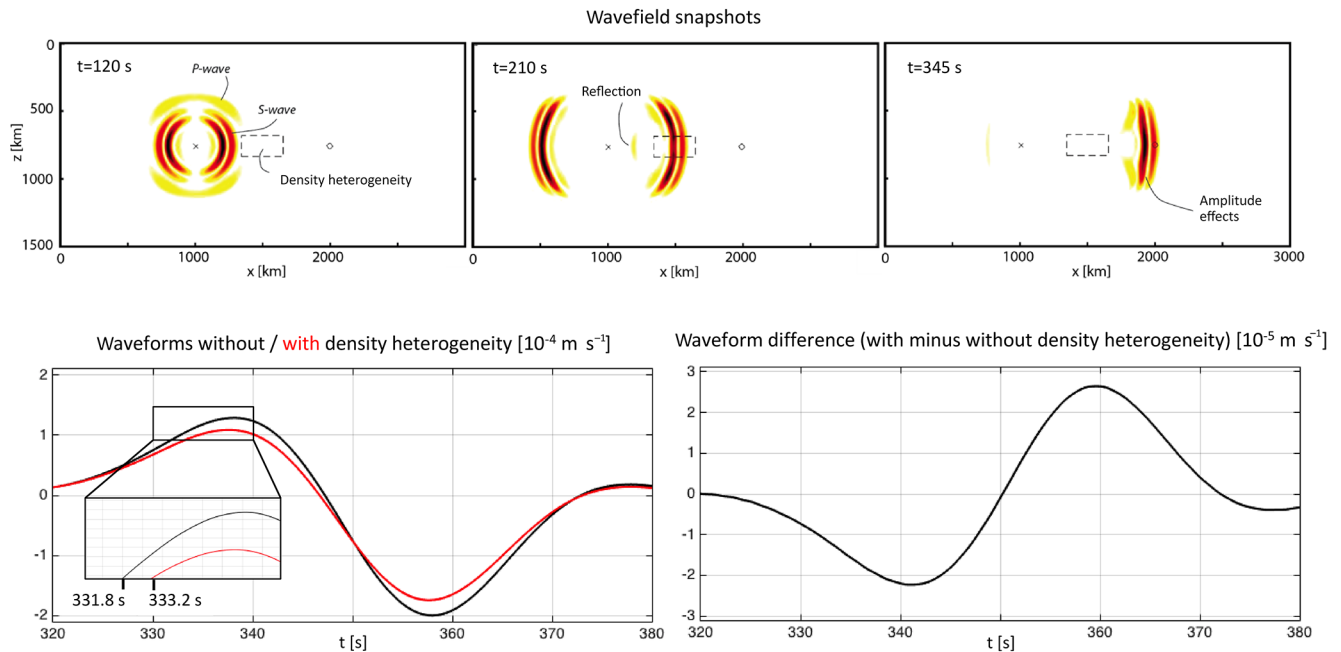
Wavefield snapshots

Waveforms without / with density heterogeneity [10^{-4} m s^{-1}]

Waveform difference (with minus without density heterogeneity) [10^{-5} m s^{-1}]

Figure 10. Illustration of finite-frequency travel-time shifts induced by a 38 % density perturbation. Top row: Wave field snapshots before, during and after the wavefront interacts with the density heterogeneity, marked by the dashed box. The interaction with the density heterogeneity causes reflections and amplitude changes of the direct wave. The onset of the wavefront, however, remains unaffected. Bottom row: Synthetic seismograms taken at the position of the black circle in the top-row snapshots. The actual onset time of the waveforms at around 320 s is identical for simulations with (red) and without (black) density heterogeneity. However, the waveform differences, plotted to the right, induce a cross-correlation time shift of $\sim$ 1 s. Locally, for example around 332 s, the time shift reaches 1.4 s.

for long-wavelength density heterogeneities especially indicates that the scattering is the dominant mechanism to produce these waveform differences. The energy transfer between the different components and towards later arrivals is also scattering-related.

As we show, the behaviour of density-induced misfits can be most often explained by an interplay of two physical parameters: the amount of scattering and the relative propagation distance. However, not all of the observed features can be interpreted on this ground. For instance, travel-time variations do not seem to exhibit a pronounced frequency-dependence, in contrast to amplitude variations that decay rapidly with decreasing frequency (see Sect. 3.2 and Fig. 6. Since the travel times of seismic waves are exactly independent of density in the infinite-bandwidth approximation of ray theory (Cerveny, 2001), the travel-time differences observed in our experiments are most likely due to finite-frequency effects. Travel-time differences measured by cross-correlation within a finite frequency band are controlled by the complex interference of direct and scattered waves, which may lead to seemingly paradoxical effects (e.g. Tong et al., 1998; Marquering et al., 1999; Dahlen et al., 2000). This may include the large negative travel-time differences shown in Fig. 7.

Figure 10 illustrates finite-frequency travel-time changes for a 2-D P-SV wave field simulation. While interacting with

a density anomaly, the wave field undergoes reflections and amplitude changes. The actual onset time of the wavefront remains largely unaffected. However, the waveform differences translate into a cross-correlation travel-time shift of $\sim$ 1 s.

We should also take into account the possible signal processing artefacts that may play a role in our analysis. In comparing between different frequency bands, we are effectively changing the bandwidth used. Therefore, some of the large time shifts that are visible in the lower frequency histogram in Fig. 6 could be a result of the existence of non-zero cross-correlation maxima for a narrow bandwidth, which would be purely signal-processing-related and have no physical interpretation. We do not expect to observe this effect in the broader frequency bands.

Naturally, scattering is a complex process that depends on the ratio of the scatterer size to the wavelength, the strength of scatterers and the source power (Groenenboom and Snieder, 1995). The signal processing artefacts and physical scattering signatures are not easily separated. Investigating whether the misfits accumulate later in the coda, which would indicate that they are scattering-related, and determining an optimal processing bandwidth size in order to decrease the amount of artificial large cross-correlation maxima, could be favourable.

The density-induced waveform differences that we found in our numerical experiments are above the noise level of many of today's regional-scale seismic recordings. While this indicates that density heterogeneities do leave a measurable imprint, it does not automatically imply that crustal density structure can be easily recovered in a tomographic inversion. Trade-offs with P and S velocity structure, for instance, may prevent the unambiguous reconstruction of density heterogeneities. The resolvability of density structure may be analysed using principal component analysis of finite-frequency kernels (Sieminski et al., 2009), and it may be improved by the construction of targeted misfit functionals (Backus and Gilbert, 1968, 1970; Bernauer et al., 2014).

Finally, we note that the amplitude of the secondary wave field scattered off density heterogeneities may have similar or smaller amplitudes than globally propagating waves, e.g. PcP, PcS or ScS. Therefore, care needs to be taken when wave propagation is modelled regionally (e.g. Cupillard et al., 2012; Gokhberg and Fichtner, 2016).

4.2 Random models of plausible Earth structure

In the absence of detailed information on crustal density structure on regional scales, we base our numerical experiments on realisations of random Earth models. To ensure that the random models are plausible, we translate rms variations in S velocity in the Anatolia model of Fichtner et al. (2013) into variations of P velocity and density, using the empirical velocity–density scaling of Brocher (2005). The plausibility of the random models is limited by three factors: (i) the variability of regional-scale rms variations in S velocity, (ii) the poorly known amplitude spectrum of velocity and density variations in the crust, and (iii) the range of different velocity–density scalings proposed in the literature. The rms variations in S velocity in the Anatolian crust are $\sim 260\,\mathrm{m\,s^{-1}}$, with a horizontal correlation length of $\sim 200\,\mathrm{km}$ and a vertical correlation length of $\sim 20\,\mathrm{km}$. These correlation lengths were used for most of the numerical experiments, except for those in Sect. 3.4, where we studied the effect of medium complexity. Similar S velocity variations on the order of $\pm 10\,\%$ over similar distances were found in tomographic studies of other regions, including the Iberian Peninsula (e.g. El Moudnib et al., 2015; Fichtner and Villaseñor , 2015), California (e.g. Shapiro et al., 2005; Tape et al., 2010), the Caribbean plate (e.g. Gaite et al., 2015), or East Asia (e.g. Chen et al., 2015). This suggests that the rms variations of S velocity variations with $200\,\mathrm{km}$ lateral and $20\,\mathrm{km}$ vertical correlation length are representative of real crustal structure at least in some regions.

For simplicity, we assume that the amplitude spectrum of the crustal velocity variations is white, meaning that velocity and density variations have nearly identical power at all scales considered in this study, i.e. from 50 to $1000\,\mathrm{km}$. The resulting velocity and density variations may be too large or too small by several percent, depending on whether a specific region is stable in the long term and subject to recent tectonic activity.

Uncertainties in velocity–density scalings are mostly caused by the natural scatter of the velocity–density relation in natural rocks. While S velocity typically varies less than $\sim 10\,\%$ for a given crustal P velocity, density can easily vary by more than $50\,\%$ for a given v_P/v_S ratio (Brocher, 2005). Despite the natural scatter, published velocity–density relationships for the continental crust as a whole show good agreement with their respective range of validity (e.g. Ludwig et al., 1970; Gardner et al., 1974; Christensen and Mooney, 1995), suggesting that the choice of a particular one does not introduce a significant bias.

In the light of these uncertainties, it must be kept in mind that the waveform variations resulting from our synthetic random density heterogeneities represent a first rough estimate. It is intended to reveal the first-order effects but not the smaller details that certainly depend on the characteristics of a specific region.

4.3 Velocity bias estimation

The shifts in travel time observed here as a result of density structure may cause a bias in velocity structure obtained in tomographic models. In order to obtain an estimate of these velocity biases, we take a simplified approach. We consider the highest frequency band from 0.02 to $0.125\,\mathrm{Hz}$ and the reference medium with 200 lateral and $20\,\mathrm{km}$ vertical correlation length, previously used in Sect. 3.3 on the effect of epicentral distance. Since we do not analyse specific seismic phases, we take the time-shift variances for different epicentral distances as representative values of time shifts induced by 3-D density structure. Furthermore, we assume that sensitivity to velocity structure is concentrated on the great circle connecting source and receiver.

Based on these simplifications, we estimate that the shear velocity bias for an epicentral distance of $200\,\mathrm{km}$ is $\sim 25\,\mathrm{m\,s^{-1}}$ or $\sim 0.78\,\%$ relative to the upper-crustal shear velocity of PREM (Dziewoński and Anderson, 1981). For epicentral distances of $1000\,\mathrm{km}$, the same bias is $\sim 21\,\mathrm{m\,s^{-1}}$ or $\sim 0.66\,\%$. It follows that the velocity biases induced by the neglect of 3-D density variations are small compared to the crustal velocity variations inferred from travel-time tomography, which are on the order of $10\,\%$. However, depending on the tomographic resolution and data quality, the biases may be larger than the error bars. A qualitative look at the detrimental effects that incorrect density information has on the wave speed models has recently been shown by Yuan et al. (2015).

4.4 Attenuation bias estimation

To quantify potential biases in attenuation induced by unknown 3-D density structure, we adopt similar simplifications as in the previous section. In the ray theory approxima-
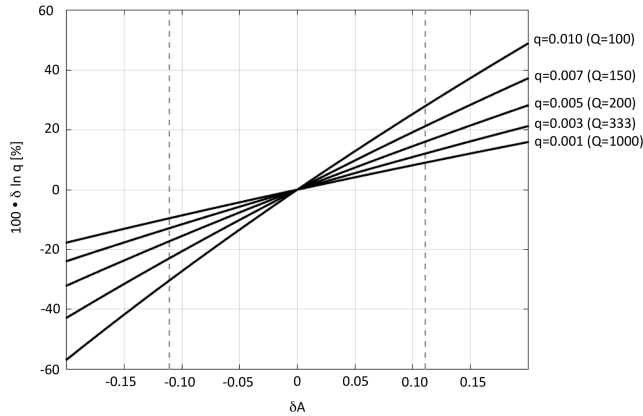
Figure 11. Fractional attenuation bias $\delta \ln q$ induced by 3-D density variations as a function of the relative amplitude difference δA. Dashed lines indicate the standard deviation of δA for the setup that we used previously to study the effect of epicentral distance (epicentral distance: 1000 km, frequency band: 0.02–0.125 Hz, lateral correlation length: 200 km, vertical correlation length: 20 km; see Sect. 3.3). The corresponding histograms are shown in Fig. 8.

tion, relative amplitude differences between attenuated and attenuation-free waves are given by

$$A = e^{\frac{-\pi r f q}{v}} \tag{4}$$

with the background attenuation or inverse quality factor denoted by q, the epicentral distance by r, frequency by f, and velocity by v. The presence of 3-D density heterogeneity induces additional relative amplitude differences, δA, that translate into apparent variations in attenuation δq,

$$A + \delta A = e^{\frac{-\pi r f (q + \delta q)}{v}}. \tag{5}$$

Combining Eqs. (4) and (5) yields the fractional apparent attenuation bias $\delta \ln q$ as a function of δA,

$$\delta \ln q = \left[\frac{\ln(A + \delta A + 1)}{\ln(A + 1)} - 1 \right]. \tag{6}$$

Equation (6) reveals that attenuation biases for a given δA have a dependence on the background attenuation q through $A = e^{\frac{-\pi r f q}{v}}$. The bias is larger for larger attenuation. Figure 11 shows fractional attenuation biases $\delta \ln q$ as a function of the background attenuation q for an epicentral distance of 1000 km, the highest frequency band from 0.02 to 0.125 Hz, and the medium with 200 km lateral and 20 km vertical correlation length. Amplitude variations for this setup are summarised in the right panel of Fig. 8.

Taking the variance of the relative amplitude differences of 0.11 as a representative value (see Sect. 3.3), the apparent variations in attenuation, $\delta \ln q$, approximately range between ±20 and ±60 % for q between 0.001 and 0.010 (Q between 100 and 1000). It follows that the apparent variations in attenuation induced by 3-D density structure can be

on the order of tens of percent, thus being comparable to attenuation heterogeneities found on regional and global scales (e.g. Mitchell, 1995; Romanowicz, 1995; Haberland and Rietbrock, 2001; Selby and Woodhouse, 2002; Dalton et al., 2008; Kennett and Abdullah, 2011; Trampert and Fichtner, 2013; Zhu et al., 2015). This result highlights that 3-D density structure should be taken into account when using full-waveform techniques to invert for 3-D variations in attenuation.

5   Conclusions

We presented a series of numerical experiments to study the effect of 3-D crustal density heterogeneities on regional seismic wave propagation in the frequency range from 0.02 to 0.125 Hz (8–50 s). These were intended to (i) reveal the extent to which density-induced waveform perturbation may be measurable, and (ii) facilitate a better intuitive understanding of the underlying wave propagation physics.

While numerical experiments can of course never be exhaustive, our series of tests still allows us to make a limited number of general statements: for media with 200 km lateral correlation length, travel-time perturbations can exceed ~ 1 s over an epicentral distance of ~ 1000 km. Amplitude perturbations for the same scenario can be several tens of percent. With decreasing frequency, amplitude perturbations decrease rapidly, but travel-time perturbations remain at approximately the same level. This indicates that the observed travel-time variations are a finite-frequency effect, i.e. a local change of amplitudes that manifests itself as a time shift, when the time shift is measured by cross-correlation.

Both amplitude and travel-time variations increase with increasing epicentral distance. This indicates that density does not only have a local effect, which is an essential prerequisite for the applicability of tomographic methods to constrain 3-D density in the crust. Waveform perturbations clearly increase with increasing medium complexity. They are practically negligible in transmission mode, i.e. when the correlation length of the medium heterogeneities is much larger than the wavelength. However, when the correlation length approaches the wavelength, density-induced waveform perturbations can be observed easily. Recent regional-scale full-waveform inversions operate in a regime where resolved heterogeneities have characteristic sizes comparable to the wavelength (e.g. Tape et al., 2010; Fichtner et al., 2013).

Our most important finding is that waveform perturbations induced by realistic crustal density variations can certainly be observed in modern, high-quality regional seismic data. While travel-time differences of typically less than 1 s will often be small compared to travel-time differences caused by velocity heterogeneities, amplitude variations of more than 10 % are comparable with those induced by 3-D velocity structure and attenuation. This implies, on the one hand, that density structure may to some extent be constrained in fu-

ture full-waveform inversions. On the other hand it suggests that current full-waveform inversions that use amplitude information may be biased due to the neglect of 3-D variations in density.

6 Data availability

The wave propagation package SES3D is a free open source software released under Apache 2.0 License. It is available for download at: http://www.cos.ethz.ch/software/ses3d. html.

The synthetic data used in this study, along with python tools for random media generation, signal comparison and histogram stacking, are to be found at: doi:10.5281/zenodo.168576, (Płonka, 2016).

Appendix A: Random model generation

We generate random media with the Fourier method, widely used in seismological research (e.g. Frankel and Clayton, 1986; Frankel, 1989; Igel and Gudmundsson, 1997; Klimeš, 2002; Jahnke et al., 2008), and recently extended to non-stationary and anisotropic media by Meschede and Romanowicz (2015). For this, we generate a random, uniformly distributed phase spectrum $\varphi(\mathbf{k})$ between $-\pi$ and π, with $\mathbf{k}$ being the 3-D wavenumber. The random spectrum $e^{i\,\varphi(\mathbf{k})}$ is then modulated by a positive, real-valued filter $f(\mathbf{k})$ to yield the wavenumber-domain random model

$$m(\mathbf{k}) = f(\mathbf{k})\, e^{i\,\varphi(\mathbf{k})}. \tag{A1}$$

The filter $f(\mathbf{k})$ is designed such that it is flat below $k_{\max}$ and wavenumber components k_i above a given threshold $k_{i,\max} = 2\pi/\lambda_{i,\min}$ are excluded. Computing the inverse Fourier transform yields the space-domain random model

$$m(\mathbf{x}) = \frac{1}{(2\pi)^3} \int\!\!\int\!\!\int m(\mathbf{k})\, e^{i\,\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{k}. \tag{A2}$$

By design, the 3-D field $m(\mathbf{x})$ only contains wavelengths above $\lambda_{i,\min}$ in the i-direction. Finally, the random realisation $m(\mathbf{x})$ is appropriately scaled and assigned to a specific medium parameter, such as density, P- or S-velocity.

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