



A computer code for forward calculation and inversion of the H/V spectral ratio under the diffuse field assumption

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ABSTRACT

During a quarter of a century, the main characteristics of the horizontal-to-vertical spectral ratio of ambient noise HVSRN have been extensively used for site effect assessment. In spite of the uncertainties about the optimum theoretical model to describe these observations, over the last decade several schemes for inversion of the full HVSRN curve for near surface surveying have been developed.

In this work, a computer code for forward calculation of H/V spectra based on the diffuse field assumption (DFA) is presented and tested. It takes advantage of the recently stated connection between the HVSRN and the elastodynamic Green's function which arises from the ambient noise interferometry theory.

The algorithm allows for (1) a natural calculation of the Green's functions imaginary parts by using suitable contour integrals in the complex wavenumber plane, and (2) separate calculation of the contributions of Rayleigh, Love, P-SV and SH waves as well. The stability of the algorithm at high frequencies is preserved by means of an adaptation of the Wang's orthonormalization method to the calculation of dispersion curves, surface-waves medium responses and contributions of body waves.

This code has been combined with a variety of inversion methods to make up a powerful tool for passive seismic surveying.

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1. Introduction

Since the early work of Kanai et al. (1954), many efforts have been devoted to the observation and interpretation of the seismic ambient noise (microtremor), consisting of background vibrations due to natural phenomena of atmospheric, oceanic, seismic and volcanic origins as well as human activities like traffic and industry. The possibility of using this ubiquitous natural illumination for exploration of ground structures with seismic arrays was soon recognized by Aki (1957).

Later, the capabilities of single-station measurements of this wavefield were enhanced by Nakamura (1989), who proposed that the ratio between the spectra of horizontal and vertical components of ambient noise allowed for identification of resonance peaks and for estimation of seismic amplifications of soils. After

these early developments, several sophisticated tools have been introduced to take full advantage of these spectral ratios for seismic exploration, which are based on diverse and in some cases opposite theoretical approaches.

Fäh et al. (2003) and Wathelet (2005) studied the inversion of the Rayleigh wave ellipticity, sometimes considered as a rough proxy of the horizontal-to-vertical spectral ratio of ambient noise (HVSRN), using genetic algorithms and the neighborhood method as inversion procedures. Their method was not intended to be applied using energy ratios of raw microtremor records, because they consist of a complicated mixture of Rayleigh, Love and body waves, but is better suited when used together with more advanced data processing aimed at extracting the ellipticity (e.g. Poggi et al., 2012).

Arai and Tokimatsu (2004) introduced a method for inversion of the HVSRN accounting for surface waves generated by a continuum of uncorrelated shallow sources located far enough from the receiver. Their approximate expressions allow for a quick and suitable estimation of the power ratio in those models and frequency bands where surface waves are the dominant contribution. Related full-wavefield versions have been developed by Lachet and

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Bard (1994) and Lunedei and Albarello (2009). To the best of the authors' knowledge, these two methods have not been incorporated into ground inversion tools. It is probably due to the intensive computing requirements.

On the other hand, a code for inversion of layered ground structures from horizontal-to-vertical spectral ratios of microtremor was published by Herak (2008). The algorithm models the HVSRL as the ratio between the ground responses for vertically incident S and P waves. In this approach, the anelastic attenuation plays a major role in order to make the H/V decay at high frequencies as observed in most experimental conditions. This can be regarded as an oversimplified scheme taking into account the predominance of surface waves found in broad frequency bands of the microtremor spectra.

Sánchez-Sesma et al. (2011) introduced an innovative method inspired in the possibility of retrieving the 3D elastodynamic Green's tensor between two stations embedded in an elastic medium from the average time-domain cross-correlation of their ambient noise records (ambient noise interferometry). Some applications of this method have been developed by Salinas et al. (2014), Kawase et al. (2015), Lontsi et al. (2015), Rivet et al. (2015), Spica et al. (2015), among others. The theoretical foundations of this general theory were developed in several research works (e.g. Snieder, 2004; Wapenaar, 2004; Sánchez-Sesma and Campillo, 2006) and confirmed in experiments with microtremors by Shapiro and Campillo (2004). The equations used here for modelling the HVSRL appear naturally in the particular case of the interstation distance tending to zero. Sánchez-Sesma et al. (2011) formulated a first algorithm for forward calculation of the HVSRL under this approach based on the discrete wavenumber integration and the matrix method described by Knopoff (1964). Equivalent results can be obtained using a generalized view of the modal equipartition proposed by Margerin (2009).

A more complete review of these theories appeared recently in Lunedei and Malischewsky (2015). The authors made a thorough description of the various theoretical models explaining the HVSRL that developed in the last three decades, including the diffuse field assumption, and compared the corresponding theoretical curves for a set of test models.

In this communication we present a faster code which allows separate computation of the contributions of SH, P-SV, Rayleigh and Love waves together with algorithms for inversion of ground structures. The software is available at the hv-inv project website <http://www.ual.es/GruposInv/hv-inv/> as FORTRAN 90 and Matlab codes. In a companion paper (Piña-Flores et al., 2016) we explore the properties of HVSRLs as well as the non-unicity problem.

2. Forward calculation of the H/V spectral ratio

The algorithms described here are based on the representation of the ambient noise wavefield as a 3D-diffuse vector field established within the medium. Then, the directional power spectral densities (PSD) of motion $P_m(\mathbf{x}; \omega)$ along any Cartesian axis m at an arbitrary point \mathbf{x} and circular frequency ω are found to be proportional to the imaginary part of the diagonal components of the Green's tensor at \mathbf{x} when both source and receiver coincide, $\text{Im}[G_{mm}(\mathbf{x}; \mathbf{x}; \omega)]$ (no sum, Sánchez-Sesma et al., 2008). When the ratio between two distinct directional PSDs is considered, the proportionality factor cancels out. Then, the ratio between the horizontal (sum of the terms associated with directions 1 and 2, which in fact are equal) and the vertical directional PSDs (term associated with direction 3), that is, the usual H/V spectral amplitude ratio at point \mathbf{x} , corresponds to:

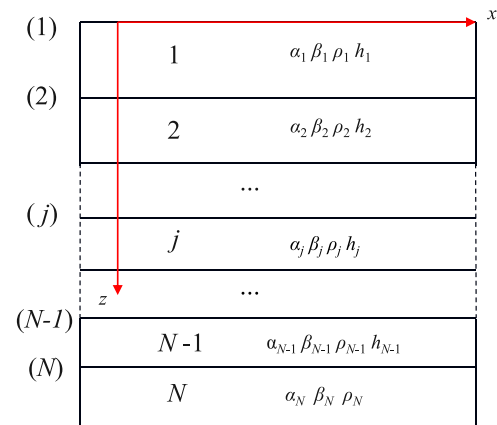


Fig. 1. Plane layered structure made of isotropic elastic layers. α_j , β_j , ρ_j and h_j stand for P- and S-wave velocities, mass density and thickness of the j -th layer. The numbering of layer and interfaces is shown.

$$[H/V](\mathbf{x}; \omega) \equiv \sqrt{\frac{2P_1(\mathbf{x}; \omega)}{P_3(\mathbf{x}; \omega)}} = \sqrt{\frac{2\text{Im}[G_{11}(\mathbf{x}; \mathbf{x}; \omega)]}{\text{Im}[G_{33}(\mathbf{x}; \mathbf{x}; \omega)]}}. \quad (1)$$

The middle expression arises from the noise auto-correlations; instead, the right hand side may be calculated theoretically under some properties and geometrical assumptions. In this work, the configuration considered is a horizontally layered structure on top of a half-space (Fig. 1). The top surface is free and the layers correspond to homogeneous, elastic and isotropic media with plane interfaces. Quantities α_j , β_j , ρ_j , $\mu_j = \rho_j \beta_j^2$ and h_j stand for P- and S-wave velocities, mass density, shear modulus and thickness of the j -th layer, respectively. Under these assumptions, a convenient way to evaluate the Green's function components in Eq. (1), on the basis of frequency-horizontal wavenumber (ω, k) representation of the wavefield, consists in using the contour integration method in the complex wavenumber plane. That method provides a rigorous way for dealing with the singularities of the original integral expressions defined on the positive k values (e.g. Harkrider, 1964).

To use the contour integration, the integrals are first extended to the whole real k axis using integrand symmetries. Then, the contour shown in Fig. 2 (Tokimatsu and Tamura, 1995; García-Jerez et al., 2013) can be employed to isolate the contributions to the Green's functions of the body and any of the surface waves modes. The body wave contributions are calculated from the integral along the branch-cuts, whereas the surface waves modes

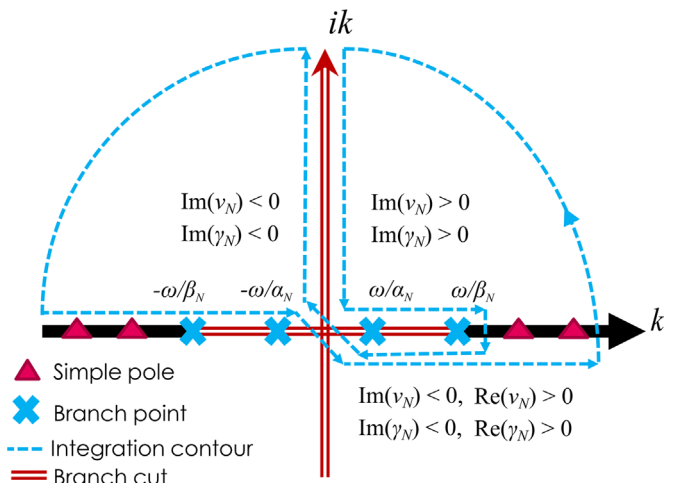


Fig. 2. Contour used for complex-plane integration, from Tokimatsu and Tamura (1995).

contributions are proportional to the residues at the poles located on the positive real k axis.

For coincident source and receiver, the sum of the branch-cut integrals along both sides of the positive imaginary axis contributes to the (diverging) real part of the Green's functions, whereas the integrals along the segments of the branch-cuts on the real axis contribute to the imaginary part. Since Eq. (1) involves $\text{Im}[G_{ij}(\mathbf{x}; \mathbf{x}; \omega)]$ only, the required numerical integration, corresponding to body waves, is constrained to the interval $[0, \omega/\beta_N]$. This may significantly speed up the computations comparing with the direct application of the conventional discrete wavenumber method, even though the actual improvement depends on the computational effort required to find the poles (dispersion curves) which varies from model to model.

The contributions of the residues at the poles and of the branch-cut integrals to the imaginary part of the Green's function at source are:

$$\begin{aligned} & \text{Im}[G_{33}(0; 0; \omega)] \\ &= -\frac{1}{2} \sum_{m \in \text{RAYLEIGH}} A_{Rm} \\ &+ \frac{1}{2\pi} \int_0^{\omega/\beta_N} \text{Re} [ik r_2(k, \omega)]_{4^{\text{th}}} dk, \end{aligned} \quad (2)$$

$$\begin{aligned} & \text{Im}[G_{11}^{PSV}(0; 0; \omega)] = \text{Im}[G_{22}^{PSV}(0; 0; \omega)] \\ &= -\frac{1}{4} \sum_{m \in \text{RAYLEIGH}} A_{Rm} \chi_m^2 \\ &+ \frac{1}{4\pi} \int_0^{\omega/\beta_N} \text{Re} [ik r_1(k, \omega)]_{4^{\text{th}}} dk, \end{aligned} \quad (3)$$

$$\begin{aligned} & \text{Im}[G_{11}^{SH}(0; 0; \omega)] = \text{Im}[G_{22}^{SH}(0; 0; \omega)] \\ &= -\frac{1}{4} \sum_{m \in \text{LOVE}} A_{Lm} \\ &+ \frac{1}{4\pi} \int_0^{\omega/\beta_N} \text{Re} [ik l_1(\omega, k)]_{4^{\text{th}}} dk, \end{aligned} \quad (4)$$

where the real quantities A_{Rm} and A_{Lm} stand for the medium responses for the m -th Rayleigh and Love modes, respectively. The expressions for the contributions of surface waves result from the limit $r \rightarrow 0$ of the general formulae derived by Harkrider (1964). The integral terms may be interpreted as the motion at surface due to wave systems for which S waves spread through the halfspace from vertically to horizontal incidence. The integrands are evaluated on the fourth-quadrant side of the real k axis. In most cases, but not always, the integrands in Eqs. (2–4) are free from poles or sharp peaks so that the computational effort for numerical integration is moderate. Some exceptions to this rule, due to the presence of leaky-mode branches in the proximity of the real k axis have been studied by García-Jerez and Sánchez-Sesma (2015).

On the other hand, it is well-known that the Thomson-Haskell propagator-matrix method presents a weakness related with numerical overflow and loss of precision at high frequencies (e.g. Buchen and Ben-Hador, 1996). Algorithms for stabilization based on Dunkin (1965) have been used in various popular codes for computation of surface waves and Green's functions (e.g. Herrmann and Ammon, 2003; Wathet, 2005). In the program described here, this question is addressed with an adaptation of the Wang's (1999) orthonormalization method, which preserves the 4×4 character of the propagators in the cases of P-SV and Rayleigh waves. The rest of this section is devoted to describe in detail the computations of the elements of Eqs. (2–4).

2.1. Computation of the surface waves contributions

2.1.1. Rayleigh waves dispersion curves

The calculation of these curves is based on the Thomson-Haskell propagator-matrix method following the formulation in Aki and Richards (2002) for propagation of plane Rayleigh waves in the x - z plane (z axis directed down).

First, the quantities $\gamma_j = \sqrt{k^2 - \omega^2/\alpha_j^2}$ and $\nu_j = \sqrt{k^2 - \omega^2/\beta_j^2}$, and the matrix L_j^{PSV}

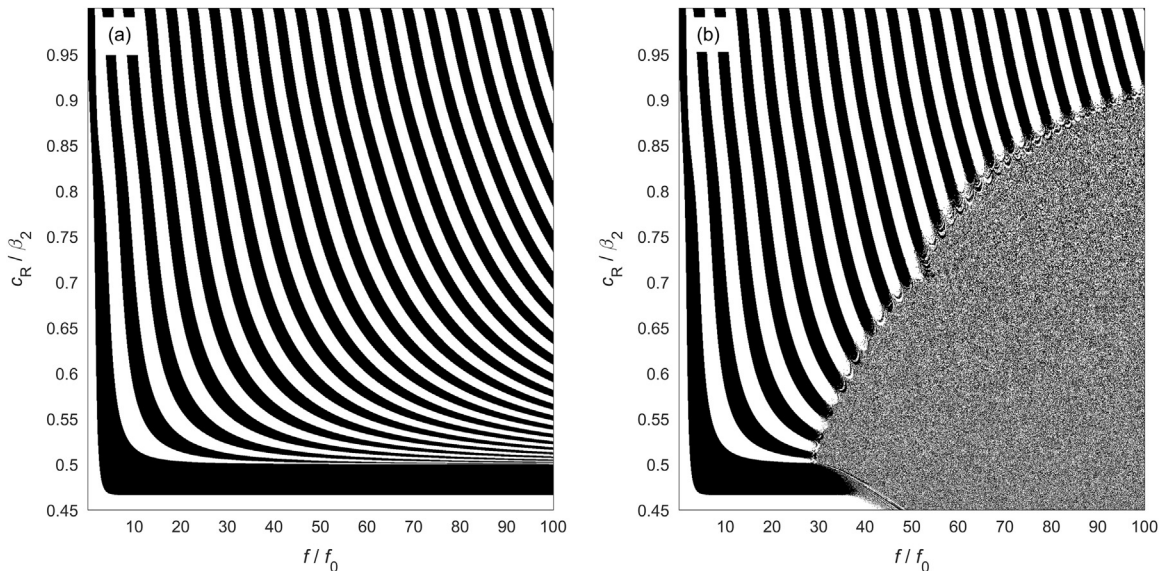


Fig. 3. (a) Sign of the determinant (frequency equation) used in this work for location of Rayleigh-waves phase velocities (Eq. 12) for an example model. Black color stands for negative and white for positive. (b) Result obtained without introducing the orthonormalization matrices Q . The model consists in a single layer over a stiffer halfspace with a contrast of 2 in β , $\alpha = 2\beta$, and no density contrast. A frequency $f_0 = \beta_1/(4h)$ is used for normalization.

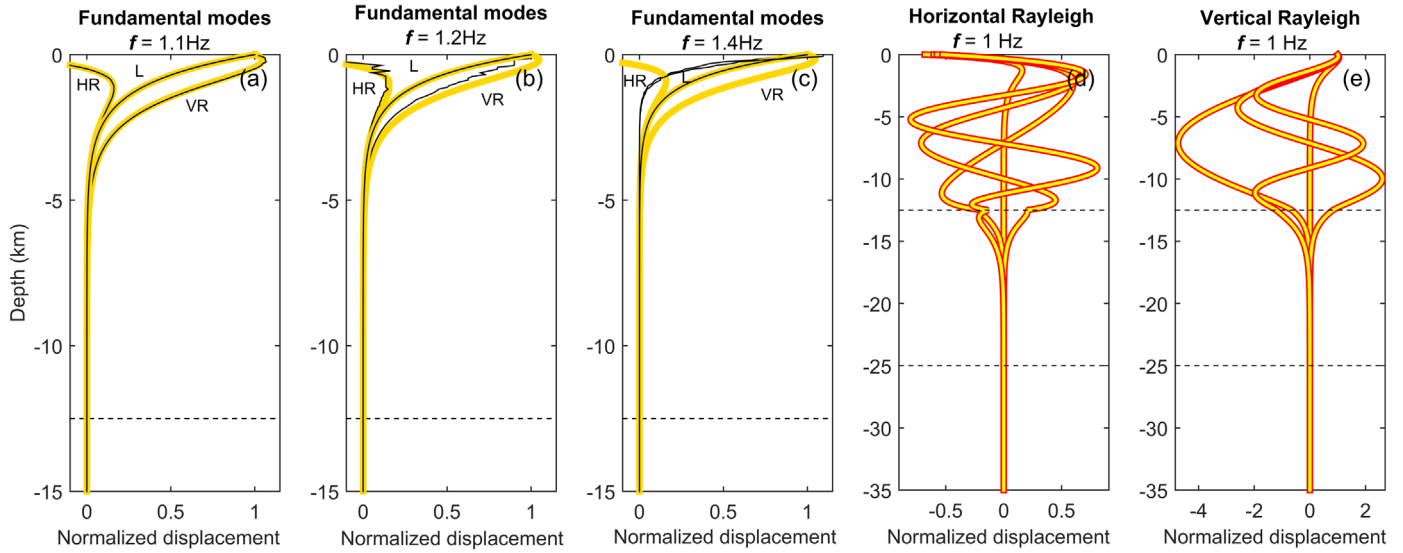


Fig. 4. (a–c) Comparison between the shapes of the fundamental mode for model 1 (Table 1), computed by means of the algorithm described in this work (yellow line) and with a non-stabilized scheme (black line) based on Aki and Richards (2002). HR, VR and L stand for Horizontal component of Rayleigh wave, Vertical component of Rayleigh wave and Love wave displacements, respectively. (d–e) Shapes of the fundamental and the first three higher modes of Rayleigh waves compared with reference curves (red lines) obtained with a global matrix method (Kausel, 2015, personal communication). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

$$L_j^{PSV} = \omega^{-1} \begin{pmatrix} \alpha_j k & \beta_j \nu_j & & & \\ \alpha_j \gamma_j & \beta_j k & & & \\ -2\alpha_j \mu_j k \gamma_j & -\beta_j \mu_j (k^2 + \nu_j^2) & & & \\ -\alpha_j \mu_j (k^2 + \nu_j^2) & -2\beta_j \mu_j k \nu_j & & & \\ & \alpha_j k & \beta_j \nu_j & & \\ & -\alpha_j \gamma_j & -\beta_j k & & \\ & 2\alpha_j \mu_j k \gamma_j & \beta_j \mu_j (k^2 + \nu_j^2) & & \\ & -\alpha_j \mu_j (k^2 + \nu_j^2) & -2\beta_j \mu_j k \nu_j & & \end{pmatrix}. \quad (5)$$

are defined for each layer. After multiplying the columns of L_j^{PSV} by $e^{-\gamma_j(z-z_j)}$, $e^{-\nu_j(z-z_j)}$, $e^{\gamma_j(z-z_j)}$ and $e^{\nu_j(z-z_j)}$, respectively and by the horizontal propagation factor $e^{i(kx-\omega t)}$, they form a basis for the waves in the j -th layer deformation-stress space $(r_1, r_2, r_3, r_4)^T = (u_x, -iu_z, \sigma_{zx}, -i\sigma_{zz})^T$ (Aki and Richards, 2002, Eq.

7.55).

Since the phase velocity of surface waves cannot be higher than β_N , the quantities γ_N and ν_N will be real. In that case, the waves within the halfspace are inhomogeneous. Taking into account these dependences on z , we first define the 4×2 coefficients matrix in the halfspace as

$$D_N = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}^T, \quad (6)$$

so that the product $Y_N^{PSV} = L_N^{PSV} D_N$ selects the two first columns of L_N^{PSV} which form a basis of the subspace of the vectors, fulfilling the radiation conditions that imply the absence of waves with unbounded amplitude at infinite depth.

To propagate this basis of the subspace upwards, fulfilling the conditions of continuity of stress and displacements across the N -th interface, Y_N is first written in terms of the full basis associated to the $(N-1)$ -th layer by means of the coefficient matrix

$$D_{N-1} = [L_{N-1}^{PSV}]^{-1} Y_N^{PSV}. \quad (7)$$

In principle, the next step would be to obtain a basis Y_{N-1}^{PSV} at the top of the $(N-1)$ -th layer as the two columns of $L_{N-1}^{PSV} E_{N-1}^{-1} D_{N-1}$, where

$$E_j^{-1} \equiv E_j(-h_j) = \begin{pmatrix} e^{\gamma_j h_j} & 0 & 0 & 0 \\ 0 & e^{\nu_j h_j} & 0 & 0 \\ 0 & 0 & e^{-\gamma_j h_j} & 0 \\ 0 & 0 & 0 & e^{-\nu_j h_j} \end{pmatrix}. \quad (8)$$

Nevertheless, when γ_j and ν_j are (positive) reals, this multiplication involves operations between the two different increasing exponentials which can cause loss of precision for a thick enough layer. Following Wang (1999), this difficulty can be avoided by means of a transformation of D_{N-1} by a 2×2 orthonormalization matrix defined as

Table 1
Example models used in this work.

h (m)	α (m/s)	β (m/s)	ρ (kg/m ³)
Model 1			
12 500	5 190	3 000	2 400
12 500	6 060	3 500	2 625
12 500	6 930	4 000	2 850
12 500	7 790	4 500	3 075
∞	8 660	5 000	3 300
Model 2			
11	1 558.8	900	2 000
12	866.0	500	2 000
12	1 212.4	700	2 000
95	1 732.0	1 000	2 000
∞	2 551.6	1 300	2 000
Model 3			
11	866.0	500	2 000
12	1 558.8	900	2 000
12	1 212.4	700	2 000
95	1 732.0	1 000	2 000
∞	2 551.6	1 300	2 000

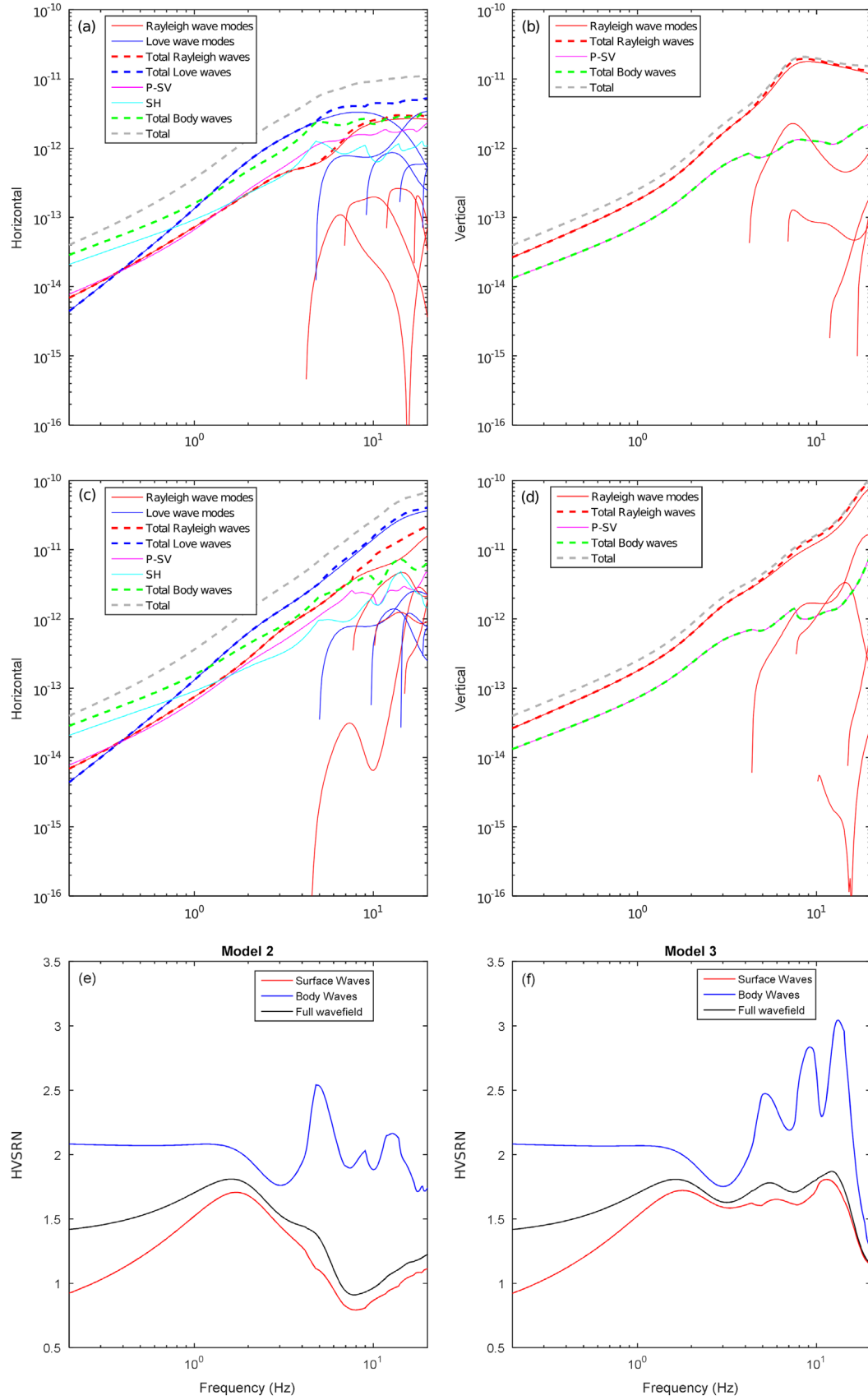


Fig. 5. Contribution of different waves to the imaginary parts of G_{11} and G_{33} for coinciding source and receiver located at surface. Panels (a) and (b) correspond to horizontal and vertical components for Model 2 (Table 1). Panels (c) and (d) correspond to Model 3. The HVSRN are shown in panels (e) and (f) for models 2 and 3, using surface waves only, body waves only and full wavefield.

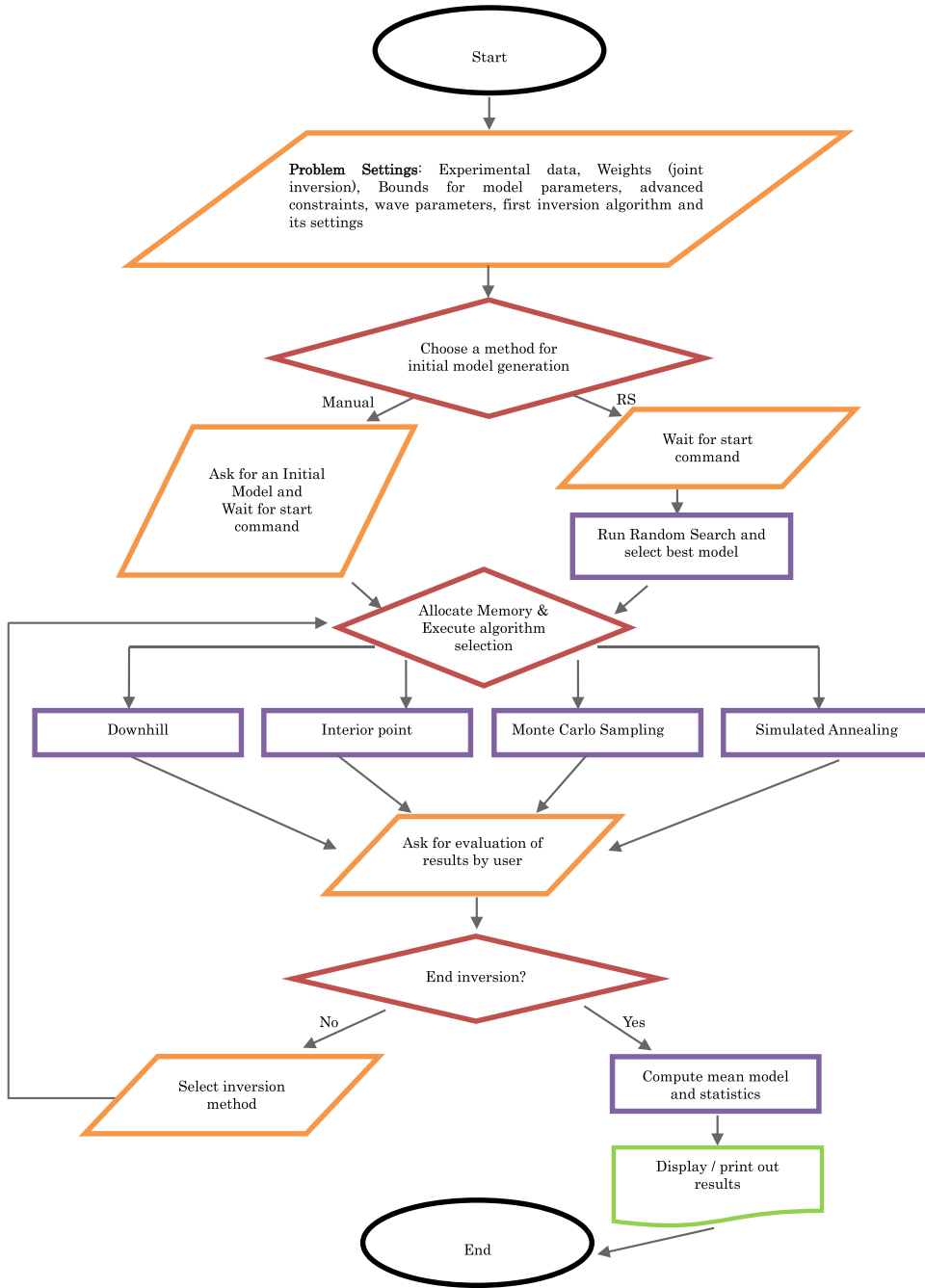


Fig. 6. Flow chart of the inversion procedure.

$$Q(D) = \frac{\begin{pmatrix} D_{22} & -D_{12} \\ -D_{21} & D_{11} \end{pmatrix}}{\sqrt{(|D_{11}|^2 + |D_{21}|^2)(|D_{12}|^2 + |D_{22}|^2)}} \quad (9)$$

Thus, $D'_{N-1} = D_{N-1}Q_{N-1}$ has zeroes at the elements 12 and 21, allowing the separation of the exponentials $e^{-\gamma_{N-1}(z-z_N)}$ and $e^{-\nu_{N-1}(z-z_N)}$ along the $(N-1)$ -th layer in the columns of $L_{N-1}^{PSV}E_{N-1}(z-z_N)D'_{N-1}$. Consequently, the alternative (stabilized) basis at z_{N-1} is:

$$Y_{N-1}^{PSV} = L_{N-1}^{PSV}E_{N-1}(-h_{N-1})D'_{N-1} = L_{N-1}^{PSV}E_{N-1}^{-1} \left\{ \left[L_{N-1}^{PSV} \right]^{-1} Y_N^{PSV} Q_{N-1} \right\}. \quad (10)$$

The procedure is then iterated up to the free surface, so that the result is formally equivalent to

$$Y_1^{PSV} = \left\{ L_1^{PSV} E_1^{-1} \left[L_1^{PSV} \right]^{-1} \right\} \left\{ L_2^{PSV} E_2^{-1} \left[L_2^{PSV} \right]^{-1} \right\} \dots \left\{ L_{N-1}^{PSV} E_{N-1}^{-1} \left[L_{N-1}^{PSV} \right]^{-1} \right\} L_N^{PSV} D_N Q_{N-1,acc} \quad (11)$$

where $Q_{j,acc} = Q_j Q_{j-1} \dots Q_2 Q_1$ stand for the accumulated transformation from the j -th layer to the surface ($Q_{N-1,acc}$ includes all the layers).

At this point, the dispersion curves could be obtained in terms of k and ω from the compatibility condition $(Y_1^{PSV})_{33} (Y_1^{PSV})_{44} - (Y_1^{PSV})_{34} (Y_1^{PSV})_{43} = 0$, which guarantees the

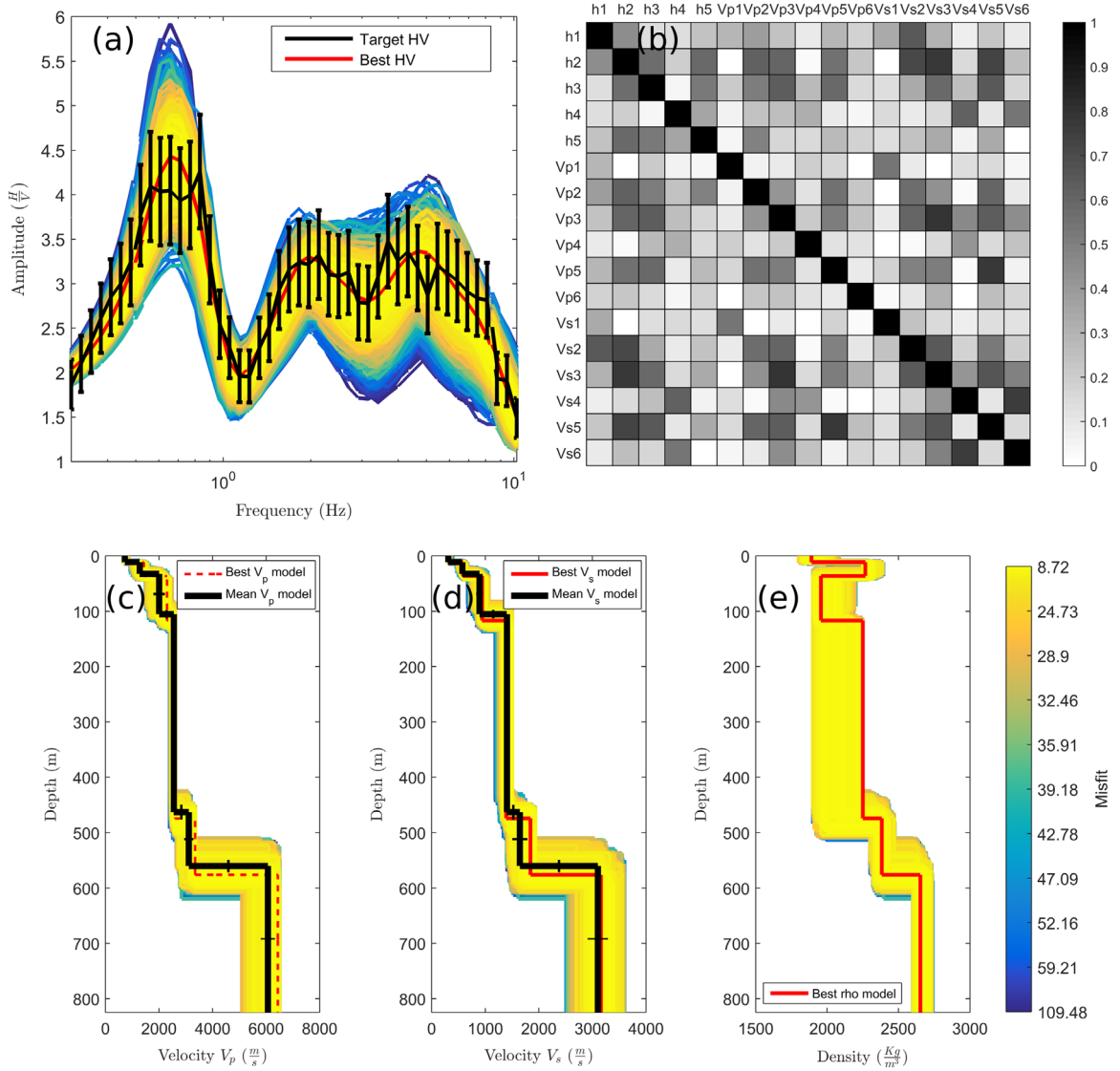


Fig. 7. Example of HVSRLN inversion for a test site (Campo de Dalías, SW Spain). Black line and black segments in panel (a) represent the experimental spectral ratio and its standard deviation. The colored curves in (a) show the forward calculations for the corresponding sampled models shown in panels (c) to (e), which were evaluated during a final application of the Monte Carlo Sampling method. Red lines show the best fitting model (panels c to e) and the corresponding theoretical HVSRLN (panel a). The mean model \mathbf{m} and the standard deviations of its parameters (C_{ij}) are shown in panels c-d with black lines, whereas panel (b) shows the normalized covariance matrix \mathbf{c} . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

existence of a non-trivial linear combination of the columns of Y_1^{PSV} fulfilling the conditions of zero stress components $\sigma_{zx}(z_1) = 0$ and $\sigma_{zz}(z_1) = 0$. Nevertheless, due to the stabilization scheme, this relation involves complex quantities $(Y_1^{PSV})_{jk}$ that would imply a more laborious root-finding task. In order to deal with real quantities, it is preferable to state an equivalent equation by using the corresponding elements of $Y_1^{PSV} Q_{N-1, acc}^{-1}$. Moreover, since any positive factor preserves the sign of the determinant and $\text{sign}[\det(Q_{N-1, acc}^{-1})] = \text{sign}[\det(Q_{N-1, acc}^*)]$, we in practice solve the equation:

$$\det \left\{ \begin{bmatrix} (Y_1^{PSV})_{31} & (Y_1^{PSV})_{32} \\ (Y_1^{PSV})_{41} & (Y_1^{PSV})_{42} \end{bmatrix} Q_{N-1, acc}^* \right\} = 0. \quad (12)$$

The signs of this expression are evaluated on the frequency-velocity plane and shown in Fig. 3a for an example model. The improvements in stability due to the orthonormalization scheme are evident in the short-wavelength region.

2.1.2. Love waves dispersion curves

The scheme followed for calculation of Love-waves dispersion curves parallels the algorithm used for Rayleigh-waves, even though the way for avoiding numerical overflow is simpler.

In this case, the out-of-plane displacement-stress vector $(l_j, l_2)^T = (u_y, \sigma_{yz})^T$ in the j -th layer can be written as the columns of

$$L_j^{SH} = \begin{pmatrix} 1 & 1 \\ -\nu_j \mu_j & \nu_j \mu_j \end{pmatrix}, \quad (13)$$

with respective dependences on $e^{i(kx - \omega t) - \nu_j(z - z_j)}$ and $e^{i(kx - \omega t) + \nu_j(z - z_j)}$. The first one is itself a basis for the harmonic waves in the half-space fulfilling the boundary conditions, so that $D_N^{SH} = (1 \ 0)^T$. Then, the iterative procedure for upwards propagation described above is applied. In this case, once the corresponding 2×1 coefficient vector for the j -th layer basis is calculated as $D_j^{SH} = [L_j^{SH}]^{-1} Y_{j+1}^{SH}$, it is subsequently normalized dividing by

$\left(\left| (D_j^{SH})_1 \right|^2 + \left| (D_j^{SH})_2 \right|^2 \right)^{1/2}$. Finally, the frequency equation arises as the zero-stress condition at the free surface: $\sigma_{yz}(z = z_1) = (Y_1^{SH})_2 = 0$.

2.1.3. Medium response for surface waves

Instead of doing a direct evaluation of the residues by using L'Hôpital's rule (see expressions in [Harkrider, 1964](#)) which requires numerical derivatives, the computations of the medium responses for surface waves modes A_{Rm} , A_{Lm} (Eqs. 3 and 4) are carried out by analytical evaluation of energy integrals along the modal shapes at pairs $(\omega, c = c_{Rm}(\omega))$ determined from the dispersion curves ([Harkrider and Anderson, 1966](#)).

According to [Section 2.1.1](#), the modal shapes for Rayleigh waves can be calculated in the j -th layer as

$$y^R(z) = L_j^{PSV} E_j(z - z_{j+1}) D_j Q_{acc, j-1} \begin{pmatrix} a \\ 1 \end{pmatrix},$$

with $z_j \leq z \leq z_{j+1}$ and $a = \frac{-(Y_1^{PSV})_{32}}{(Y_1^{PSV})_{31}}$. (14)

The modal index m and the layer index j in $y^R(z)$ are dropped off for the sake of simplicity. The multiplication by $(a \ 1)^T$ in [Eq. \(14\)](#) generates a linear combination of the basis Y_1^{PSV} that fulfils the zero-stress condition at surface, whereas the multiplication by $Q_{acc, j-1}$ transforms D_j into the surface basis Y_1^{PSV} (since no transformation is required for z within the first layer, $Q_{acc, 0}$ can be defined as the identity matrix). The modal shapes of Love waves can be computed using an analogous (but simpler) scheme.

The calculation described above has been checked in many test models, showing accuracy and stability. [Fig. 4d–e](#) show the perfect matching with the results of a global matrix method for the model defined by [Denolle et al. \(2012\)](#) in similar tests (Model 1 in [Table 1](#)). An example of the instability of the original propagator matrix method as frequency grows is shown in [Fig. 4a–c](#) (black lines).

This scheme is subsequently used to compute the integrals ([Ben-Menahem and Singh 2000](#), Eq. 3.139) for Rayleigh wave modes:

$$I_0^R = \sum_{j=1}^N \rho_j \int_{z_j}^{z_{j+1}} \left\{ |u_x(z)|^2 + |u_z(z)|^2 \right\} dz, \quad (15)$$

$$I_1^R = \sum_{j=1}^N \mu_j \int_{z_j}^{z_{j+1}} \left\{ \frac{\alpha_j^2}{\beta_j^2} |u_x(z)|^2 + |u_z(z)|^2 \right\} dz \quad (16)$$

and

$$I_3^R = \sum_{j=1}^N \mu_j \int_{z_j}^{z_{j+1}} \left\{ \frac{\alpha_j^2}{\beta_j^2} \left| \frac{du_z(z)}{dz} \right|^2 + \left| \frac{du_x(z)}{dz} \right|^2 \right\} dz, \quad (17)$$

where $u_x(z) = r_1(z)$ and $u_z(z) = i r_2(z)$ refer to the displacement components of the modal vector $y^R = (r_1, r_2, r_3, r_4)^T$.

Then, the group velocity is calculated from these integrals and from the phase velocity c_R as

$$v_{gR} = \frac{c_R^2 I_0^R - c_R^2 I_3^R / \omega^2 + I_1^R}{2 I_0^R c_R}, \quad (18)$$

which can be worked out from [Ben-Menahem and Singh \(2000](#), Eqs. 3.139, 3.140, 3.141 and 5.128). Note that numerical derivatives of the phase-velocity dispersion curves are avoided in this way. Then, the medium response is subsequently computed as

$$A_R = \frac{|u_z(z_1)|^2}{2 v_{gR} c_R I_0^R}. \quad (19)$$

In the case of Love waves, the relevant energy integrals to be evaluated are

$$I_0^L = \sum_{j=1}^N \rho_j \int_{z_j}^{z_{j+1}} |u_y(z)|^2 dz \quad (20)$$

and

$$I_1^L = \sum_{j=1}^N \mu_j \int_{z_j}^{z_{j+1}} |u_y(z)|^2 dz \quad (21)$$

whereas the medium response can be worked out as:

$$A_L = \frac{|u_y(z_1)|^2}{2 I_1^L} \quad (22)$$

([Ben-Menahem and Singh 2000](#), Eqs. 3.128, 3.129 and 5.126). For joint inversion purposes, the group velocity of Love waves can also be calculated as

$$v_{gL} = \frac{I_1^L}{I_0^L c_L}. \quad (23)$$

Since calculations of medium responses are independent for each frequency and mode, the computation can be easily parallelized to improve performance in shared memory multiprocessing systems. In this manner, each thread deals with a subset of frequencies. This feature has been implemented by means of OpenMP constructs. This also applies to the body wave contributions.

2.2. Computation of body waves contributions

The last step is to evaluate the integral terms in [Eqs. \(2–4\)](#), which address the effects of the diffuse P-SV and SH body wave-field, respectively. Thus, for any fixed ω and for both P-SV and the SH contributions, the wavenumber k is uniformly varied from 0 to ω/β_N , corresponding to outgoing S waves spreading from vertically to horizontally in the halfspace. The P waves in the halfspace can either be of homogeneous or inhomogeneous type.

For each couple (ω, k) , the boundary conditions at the halfspace and the continuity of stress and displacements through the structure are stated, except at the *source* (evaluation point) located at surface. In particular, respective bases for the displacement-stress vectors $(r_1, r_2, r_3, r_4)^T$ and $(l_1, l_2)^T$ at $z = 0$ are generated by following procedure in [Eq. \(6–11\)](#) for P-SV waves, and that in [Section 2.1.2](#) for SH waves.

The constant factors in [Eqs. \(2–4\)](#) have been fitted to represent discontinuities δr_3 , δr_4 and δl_2 corresponding to unitary forces, that is, $\delta r_4 = F_z = 1$, and $\delta r_3 = \delta l_2 = F_x = 1$. These factors can be derived from the more general formulation in [Aki and Richards \(2002\)](#), who describe the discontinuities in r_4 , r_3 and l_2 by means of the functions $f_R(k, m)$, $f_S(k, m)$ and $f_T(k, m)$. The particular cases of point forces acting in directions z and x are described by $f_R(k, m = 0) = F_z$, $f_S(k, m = 1) = -F_x/2 = -f_S(k, m = -1)$, and $f_T(k, m = 1) = iF_x/2 = f_T(k, m = -1)$. These functions vanish for any other value of m .

Therefore, to obtain the body-wave terms of G_{33} , a linear combination of the vectors $(Y_1^{PSV})_{j1}$ and $(Y_1^{PSV})_{j2}$ fulfilling the system of equations $(r_1, r_2, 0, \delta r_4)^T = Y_1^{PSV}(a, b)^T$ has to be found. The coefficients (a, b) can be worked out from the third and fourth equations and used to write the factor $r_2(\omega, k)$ of the integrand as

$$r_2(\omega, k) = \frac{(Y_1^{PSV})_{31}(Y_1^{PSV})_{22} - (Y_1^{PSV})_{32}(Y_1^{PSV})_{21}}{(Y_1^{PSV})_{31}(Y_1^{PSV})_{42} - (Y_1^{PSV})_{41}(Y_1^{PSV})_{32}}, \quad (24)$$

where F_z has been replaced with 1. To obtain the contributions of P and SV waves to the radial motion, $r_1(\omega, k)$ is worked out from $(r_1, r_2, \delta r_3, 0)^T = Y_1^{PSV}(a, b)^T$. Proceeding as in the previous case, it results:

$$r_1(\omega, k) = \frac{(Y_1^{PSV})_{42}(Y_1^{PSV})_{11} - (Y_1^{PSV})_{41}(Y_1^{PSV})_{12}}{(Y_1^{PSV})_{31}(Y_1^{PSV})_{42} - (Y_1^{PSV})_{41}(Y_1^{PSV})_{32}}. \quad (25)$$

Finally, in the case of SH waves, the system of equations to be solved is $(l_1, \delta l_2)^T = Y_1^{SH} a$, with $\delta l_2 = \delta \sigma_{zx} = F_x = 1$. The solution is:

$$l_1 = a(Y_1^{SH})_1 = \delta l_2(Y_1^{SH})_1 / (Y_1^{SH})_2 = (Y_1^{SH})_1 / (Y_1^{SH})_2 \quad (26)$$

To illustrate the computations of surface-waves and body-waves parts of $\text{Im}[G_{jj}(0; 0; \omega)]$, we show the individual contributions of each type of wave for several shallow models listed in Table 1. Models 2 and 3 (called M5 and M6 in Pei, 2007) consist of three thin layers (35 m total) overlying a thicker fourth layer (95 m). These two models present low and high velocity zones in the second layer, respectively, and the velocity contrasts are moderate.

As shown in Fig. 5, the horizontal component is dominated by surface waves from 0.7 Hz in both models, with Love waves being the main component. SH waves are the main contribution at lower frequencies. For Model 3, the fundamental Love mode dominates the surface wavefield, whereas the first higher mode becomes the dominant Love mode at 14.5 Hz for Model 2, with Rayleigh waves being the main contribution in a narrow transition band around this frequency. The vertical component is dominated by Rayleigh waves of the fundamental mode in both models. As shown in Fig. 5e–f, the surface waves control the overall shape of the HVSRN except for frequencies below the fundamental SH resonance of the model. Resonances of body waves also introduce some bumps in the H/V ratio, such as the visible SH resonance at 4.9 Hz for Model 2. In spite of the smaller effects on the overall shape of the spectral ratio, the computation of body wave contributions is often the most time-consuming part of the forward problem. For example, between 5000 and 10000 evaluations of the integrand were carried out to obtain a perfect estimation of SH and P-SV terms for Model 3 in the frequency ranges shown in Fig. 5. Those integrals consumed the 91–97% of the total computing time. In inverse problem, the user may assess the appropriateness of neglecting body wave contributions to speed up repetitive forward calculations on the basis of an *a priori* estimation of the ground model and considering the size of the experimental uncertainties.

It should be noted that the models consider here are purely elastic. However, it is known that pronounced viscoelasticity, which is often found in shallow structures, may considerably change the properties of seismic waves. Our experiments based on simple models with high impedance contrasts (e.g. Sánchez-Sesma et al., 2011; Salinas et al., 2014; Sánchez-Sesma, 2016) show that the main effect of the anelastic attenuation is the decreasing of the main peak amplitude as the quality factor decreases. For example, Sánchez-Sesma (2016) has reported a decrement of 23% in amplitude at the peak for a quality factor of 200. Contrary to some other approaches (Herak, 2008), the effects of attenuation were almost negligible at higher frequencies, at which the Green's functions are dominated by surface waves, and the effects on the overall shape remain moderate.

3. Inversion of HVSRN and of surface wave velocities

In a general sense, the inversion of geophysical data consists in finding properties of the so called *a posteriori* probability distribution, which measures the probability of any model \mathbf{m} (a ground profile) of being the true model on the basis of its ability to fit a set of observations $d_j^{obs} \pm \sigma_j$ and fulfilling *a priori* constraints. The method for forward calculation, $d_j^{theo}(\mathbf{m})$, is assumed to be known. Most of the applications are intended to characterize this probability distribution by means of the maximum likelihood model, the mean (expected) model and/or the covariance matrix for the model parameters.

The inversion software provided here has been written in Matlab[®] and includes implementations of three main inversion algorithms: i) Monte Carlo sampling ii) the Simulated Annealing method (SA) and iii) the Interior Point method (IP), together with a suitable graphic user interface. In addition, two simpler methods such as the Random Search (RS) and the Downhill-Simplex are also available. These methods can be sequentially applied following the program flow chart sketched in Fig. 6.

The interface allows both independent and joint inversion of HVSRN and Rayleigh- or Love-wave phase or/and group velocities. Since only variations in the elastodynamic properties with depth are considered, our procedure requires that the structure beneath the experimental setting may be locally approximated by a horizontally layered medium. If the dataset includes surface wave velocities and HVSRNs, the similarity among the spectral ratios for all the stations of the array used for dispersion curve retrieval can be stated as a consistency control. The main features of these implementations are described in this section.

3.1. Random search

A random search on the model space can be performed alone or as a first stage of a more complicated inversion procedure. The user has to set up suitable intervals for the ground parameters (α_j , β_j , ρ_j , h_j and Poisson's ratios) as *a priori* information. Uniform probability is assumed for layer thicknesses and densities within the stated ranges as well as for either α_i or β_i , depending on the program settings. The remaining velocity type is also uniformly sampled even though the actual range could be made narrower to be compatible with the Poisson's ratio intervals. In addition, it is possible to impose downward-increasing $\alpha(z)$ or $\beta(z)$ velocity profiles. Instead of rejecting invalid profiles among the random models, the semi-analytical approach described in Appendix A has been followed to implement these constraints.

After a number of trials defined by the user, the model presenting the lowest value of the misfit, $E(\mathbf{m})$, defined as

$$E(\mathbf{m}) = \sum_j (d_j^{obs} - d_j^{theo}(\mathbf{m}))^2 / \sigma_j^2 \quad (27)$$

is selected. For joint inversion of an HVSRN together with a dispersion curve, Eq. (27) is slightly generalized to

$$E(\mathbf{m}) = 2(1-w_c) \sum_{j=1}^{n_{HV}} \left(\frac{HV_j^{obs} - HV_j^{theo}(\mathbf{m})}{\sigma_{HVj}} \right)^2 + 2w_c \sum_{j=1}^{n_c} \left(\frac{c_j^{obs} - c_j^{theo}(\mathbf{m})}{\sigma_{cj}} \right)^2, \quad (28)$$

where n_{HV} and n_c are the respective number of samples and an adjustable weight parameter w_c ranging from 0 to 1 controls the relative weight of the dispersion curve in the global misfit. The default choice of $w_c = 0.5$ guarantees the same weight for all the samples, regardless of the observable they represent. On the

contrary, w_c can be used to equalize the sensitivity of $E(\mathbf{m})$ to spectral ratios and velocities, which could be retrieved for a very different number of samples. To do so, the software provides the option of making an inverse weighting fulfilling $w_{HV}/w_c = n_c/n_{HV}$, where w_{HV} represents $(1 - w_c)$. In particular, it takes $w_c = \frac{n_{HV}}{n_{HV} + n_c} = \frac{n_{HV}n_c}{n_{HV} + n_c} \frac{1}{n_c}$, so that $w_{HV} = \frac{n_{HV}n_c}{n_{HV} + n_c} \frac{1}{n_{HV}}$. In the case of coinciding n_{HV} and n_c then w_c and w_{HV} equal 0.5 and the unweighted expression (27) is recovered.

3.2. Simulated Annealing and Monte Carlo sampling

The SA inversion method (Kirkpatrick et al., 1983) is inspired in the process of heating a solid until it melts and then cooling very slowly until the substance reaches the state of lowest energy, forming a perfect crystal. This technique uses the Metropolis algorithm (Metropolis et al., 1953; Hastings, 1970) to sample the model space M with a Gibbs-type probability density function

$$G(\mathbf{m}, T) = \exp\left(\frac{-E(\mathbf{m})}{T}\right) / \int_M \exp\left(\frac{-E(\mathbf{m})}{T}\right) d\mathbf{m}. \quad (29)$$

In Eq. (29), $E(\mathbf{m})$ resembles the energy, and T a fixed value which is decreased slowly and corresponds to the temperature in the thermodynamic analog (the Boltzmann constant is taken equal to one).

The cooling schedule, defined by the number of temperatures, its initial value and reduction ratio as well as the number of model per temperature (Markov's chain length) are set by the user. In addition to the best fitting model, the software computes the mean model $\bar{\mathbf{m}}$, its uncertainties and the normalized covariance matrix \mathbf{C} for a set of iterations performed at the lower temperature reached. The relevant formulae are:

$$\bar{\mathbf{m}} = \int_M \mathbf{m} G(\mathbf{m}) d\mathbf{m} \quad (30)$$

and

$$c_{ij} = |c_{ij}| / \sqrt{c_{ii}c_{jj}}, \quad \mathbf{C} = \int_M (\mathbf{m} - \bar{\mathbf{m}})(\mathbf{m} - \bar{\mathbf{m}})^T G(\mathbf{m}) d\mathbf{m}, \quad (31)$$

where \mathbf{m} is written as a column/ce: bold> is written as a column vector. Since the model space is sampled according to the distribution $G(\mathbf{m})$, the integrals turn into the unweighted averages of \mathbf{m} and $(\mathbf{m} - \bar{\mathbf{m}})(\mathbf{m} - \bar{\mathbf{m}})^T$ respectively, over the set of models obtained in this way.

This method has been successfully used for inversion of surface-waves dispersion curves by Iglesias (2000) and Pei et al. (2007) among others. Comparisons between the SA and two more heuristic methods as well as with linearized inversion have been carried out by Yamanaka (2005) and Pei (2007), respectively. Yamanaka's numerical experiments showed that SA provides a rapid convergence and finds models with the smallest misfits.

With the above definition of $E(\mathbf{m})$, the *a posteriori* probability density in the case of independent Gaussian uncertainties is proportional to $P(\mathbf{m}, T = 2)$. The exploration at this constant temperature is implemented as a separate option of the software and referred to as Random Monte Carlo sampling (e.g. Mosegaard and Tarantola, 1995). In this case, $\bar{\mathbf{m}}$ and c_{ij} calculated from Eqs. (30 and 31) have a clear statistical meaning. Note that the introduction of the decreasing temperature in the SA method can be thought as a way of distorting the *a posteriori* probability distribution until it sharply peaks at the maximum likelihood (minimum energy) model (Tarantola, 2005). In this way, the neighborhood of this model is virtually the only sampled region at the end of the cooling process.

3.3. Local optimization methods

The built-in implementation of the interior-point method for non-linear constrained optimization (e.g. Waltz et al., 2006) usually converges faster than the SA algorithm (and much faster than the RS) to a minimum of $E(\mathbf{m})$. Since it is prone to converge to local minima, this algorithm would be suitable when the a priori information allows for significant restrictions of the model space (encoded by the user) or when the solution is known to be well approximated by the initial model. This method also performs well for joint inversion of HVSr and dispersion curves, due to the implied reduction of the set of equivalent solutions (see Piña-Flores et al., 2016 for further discussion on non-unicity).

The procedure is based on the Matlab implementation of this method through *fmincon* command, which attempts to find the minimum of constrained nonlinear multivariable functions. The user has to set up the termination criterion in terms of minimum meaningful variations in model parameters and misfit decrements. The maximum number of iterations and misfit evaluations can also be limited. The bounds imposed to the model parameters as well as the optional constraints related with increasing $\alpha(z)$ or $\beta(z)$ functions are coded by means of the inequalities which define the constraints in this optimization method.

A basic implementation of the downhill simplex method (Nelder and Mead, 1965) based on a built-in Matlab procedure has also been incorporated to the interface. Even though this derivative-free algorithm is aimed at unconstrained minimization problems, the ground model constraints are taken into account through misfit penalization of models for which they are violated. The speed of this method is very good for low and moderate model space dimensionality.

4. Test with real data

The reliability of H/V ratios obtained under the diffuse field assumption has been already stated by Sánchez-Sesma et al. (2011) and Salinas et al. (2014) among others. These two studies deal with H/V curves of relatively simple shape associated with resonances of a shallow soft layer (as soft as 70 m/s for β_1). In this section, the outputs of the presented software and its suitability are illustrated for a sample HVSrN measured in a very different environment.

The measurements used here were performed in the context of seismic investigations in Campo de Dalías, a large coastal plain in SW Spain and correspond to a test site located at El Ejido town. Previous active multichannel seismic surveys and borehole analysis revealed the stratigraphic record in the vicinity of the measurement point. The shallow layers are formed by anthropogenic fillings of insignificant thickness overlying Pliocene materials (calcarenes, silts and marly limestones). The Pliocene-aged layer is underlain by the thickest Neogene unit, of Messinian age (Pedrera et al., 2015), and composed at its base of lower Messinian silts and marls overlain by gypsum layers, marly limestones and silts. An older and thinner layer made up of late Tortonian calcarenites and conglomerates rests on the basement, which is attributed to the Permo-Triassic metamorphic rocks of the Alpujárride Complex (Betic Cordillera).

We used a CMG-6TD broad-band seismometer. The recording time was of 30 minutes and the sampling rate was 100 sps. Traces were first divided in a set of overlapping windows of 40.48 s. Then, the HVSrN was calculated following the procedure stated by Sánchez-Sesma et al. (2011), which involves normalization of each time window by its total energy, calculation of the power spectral density for each component and the subsequent computation of the spectral ratio according with Eq. (1). The H/V curve (black line

in Fig. 7a) shows a somewhat complicated shape with a clear main peak at 0.65–0.7 Hz and a broad secondary bump between 1.3 and 8.0 Hz, approximately. In turn, at least a pair of minor peaks can be identified in that latter band.

The inversion has been performed combining SA with the local methods. The allowed ranges for the ground parameters α and ρ were based on previous work performed by Marín-Lechado (2005) in Campo de Dalías. Once a good fitting of the data was obtained, 4000 more models were generated by Monte Carlo sampling to compute the mean model, the standard deviation and the covariance matrix (Fig. 7). The obtained model is consistent with the information available from previous studies. For example, the two-way P-wave travel time down to the bottom of the layer interpreted as Messinian marls (418 ms) agrees very well with the corresponding value derived from active-source seismic methods (Plata-Torres et al., 2004, p. 164), and the depth of the basement matches the results obtained by González et al. (2003).

5. Concluding remarks

An algorithm for forward calculation of HVSRN based on the diffuse field approximation (Sánchez-Sesma et al., 2011) has been described and implemented in a FORTRAN 90 code. This method provides a full-wavefield interpretation of this observable and it is compatible with the recent developments in ambient noise interferometry.

An orthonormalization technique has been used to preserve the stability of the code at high frequency, preventing from underflow/overflow problems in the susceptible steps of the algorithm: computation of dispersion curves, medium responses to surface-wave modes and contribution of body waves.

The separate calculation of each contribution to the wavefield allows a better understanding of the physics. Moreover, it would make feasible to state corrections in cases of deviations of the wavefield composition from the energy ratios stated by the equipartition principle. Examples of this behavior have been reported by Nakahara and Margerin (2011) among others.

This code has been incorporated into a program for inversion of HVSRN which supports joint inversion of the spectral ratio and the surface waves dispersion curves. This approach has been demonstrated to reduce the tradeoff between thicknesses and velocities inherent to inversion of H/V ratios and improves the sensitivity to velocity contrasts of profiles obtained from dispersion curves, and in particular to the basement velocity (e.g. Arai and Tokimatsu, 2005; Parolai et al., 2005; Piña-Flores et al., 2016). The program allows for applying Monte Carlo sampling of the model space, the SA algorithm as well as local methods. The numerical calculation of the body waves integrals is often the most time-consuming part of the forward problem, even though these terms often have minor effects on the HVSRN curves. In very intensive problems, the software can be used for doing a preliminary inversion based on surface-waves components, letting final refinements with full wavefield computations for a second stage.

The application of this software to real data obtained at a moderately deep sedimentary structure provided good fitting of the experimental curve, including secondary peaks and features. The results were consistent with previous information obtained from boreholes and conventional seismic methods.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at <http://dx.doi.org/10.1016/j.cageo.2016.06.016>.

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