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P-SV multimode summation differential seismograms for layered structures: extension to high frequencies and oceanic structural models

Summary – Differential seismograms with respect to structural model parameters can be computed analytically using the multimode summation formalism for laterally homogeneous layered media [1]. To calculate differential seismograms, partial derivatives with respect to structural model parameters of eigenfunctions, energy integral, phase and group velocity are needed.

We extend the existing formalism and related computer codes to evaluate: (1) differential seismograms in case of oceanic structural models, and (2) partial derivatives of group velocity for frequencies greater than 0.05Hz.

Key words: differential seismograms, multimode summation, partial derivatives.

1. Differential seismograms and partial derivatives

An analytical method for computing differential seismograms with respect to structural model parameters is given in [1]. The method adopted the P-SV-wave multimode summation formalism for laterally homogeneous layered media [7], [8], [9].

The displacement for a double-couple point source and for a given Rayleigh mode can be expressed in the frequency domain [6] as:

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$$U_r(\omega) = R(\omega)|\mathrm{n}|k^{1/2} \exp\left(\frac{-i3\pi}{4}\right)\chi(\Theta,h)\varepsilon_0 E \frac{\exp(-ikr)}{(2\pi\ r)^{1/2}} \tag{1}$$

$$U_z(\omega) = \left[\varepsilon_0 \exp\left(\frac{i\pi}{2}\right)\right]^{-1} U_r(\omega) \tag{2}$$

where R(ω) is the Fourier transform of the equivalent point-force time function, χ is the source radiation pattern, n is the unit vector perpendicular to the fault surface and has units of length, k is the wave number, r is the epicentral distance, and $\varepsilon_0 = u^*(0)/w(0)$ ($u^* = Im(u)$) is the ellipticity calculated as the ratio of the radial and vertical components $u(z)$ and $w(z)$ of the Rayleigh-mode eigenfunctions at the free surface. The factor E is given by

$$E = \frac{1}{2cUI_1} \tag{3}$$

where c and U are the phase and group velocities respectively. The energy integral is defined as

$$I_1 = \int_0^\infty \varrho(z)\left\{\left[\frac{w(z)}{w(0)}\right]^2 + \left[\frac{u^*(z)}{w(0)}\right]^2\right\}dz \tag{4}$$

where $\varrho(z)$ is the density. For a double-couple point source [4] the source radiation pattern is

$$\chi(\Theta,\mathrm{h}) = \mathrm{d}_0 + \mathrm{i}(\mathrm{d}_1\sin\Theta + \mathrm{d}_2\cos\Theta) + \mathrm{d}_3\sin2\Theta + \mathrm{d}_4\cos2\Theta \tag{5}$$

$$\begin{aligned}
\mathrm{d}_0 &= \frac{1}{2}\mathrm{B(h)}\sin\lambda\ \sin2\delta \\
\mathrm{d}_1 &= -\mathrm{C(h)}\sin\lambda\ \cos2\delta \\
\mathrm{d}_2 &= -\mathrm{C(h)}\cos\lambda\ \cos\delta \\
\mathrm{d}_3 &= \mathrm{A(h)}\cos\lambda\ \sin\delta \\
\mathrm{d}_4 &= -\frac{1}{2}\mathrm{A(h)}\sin\lambda\ \sin2\delta
\end{aligned} \tag{6}$$

Θ is the angle between the strike of the fault and the epicentre-station direction, λ is the rake angle, δ is the dip angle and h is the source depth. A(h), B(h) and C(h) depend on the eigenfunctions at the source depth

$$A(h) = -\frac{u^*(h)}{w(0)}$$

$$B(h) = -\left[3\text{-}4\,\frac{\beta^2(h)}{\alpha^2(h)}\right]\frac{u^*(h)}{w(0)} - \frac{2}{\varrho(h)\alpha^2(h)}\,\frac{\sigma^*(h)}{\dot{w}(0)/c} \tag{7}$$

$$C(h) = -\frac{1}{\mu(h)}\,\frac{\tau(h)}{\dot{w}(0)/c}$$

where the dot indicates time differentiation and σ and τ are the normal and tangential stresses, respectively.

To compute the differential seismograms with respect to the structural parameters we need to compute the partial derivatives of the terms in equations (1) and (2) that depend on the structural parameters, namely

$$\varepsilon_0, \qquad \chi(\Theta,h), \qquad E = \frac{1}{2cUI_1}, \qquad k^{1/2}, \qquad \exp(\text{-}ikr) \tag{8}$$

Using the partial derivatives of the terms (5) the differential seismograms can be computed according to the following expressions

$$\frac{\partial}{\partial p_j}U_r(\omega) = U_r(\omega)\left[\frac{1}{\chi(\Theta,h)}\frac{\partial}{\partial p_j}\chi(\Theta,h) - \left(\frac{1}{c}\frac{\partial c}{\partial p_j} + \frac{1}{u}\frac{\partial u}{\partial p_j} + \frac{1}{I_1}\frac{\partial I_1}{\partial p_j}\right)\right.$$
$$\left. + \left(\frac{1}{2k} - i\cdot r\right)\frac{\partial k}{\partial p_j} + \frac{1}{\varepsilon}\frac{\partial \varepsilon_0}{\partial p_j}\right] \tag{9}$$

$$\frac{\partial}{\partial p_j}U_z(\omega) = U_z(\omega)\left[\frac{1}{\chi(\Theta,h)}\frac{\partial}{\partial p_j}\chi(\Theta,h) - \left(\frac{1}{c}\frac{\partial c}{\partial p_j} + \frac{1}{u}\frac{\partial u}{\partial p_j} + \frac{1}{I_1}\frac{\partial I_1}{\partial p_j}\right)\right.$$
$$\left. + \left(\frac{1}{2k} - i\cdot r\right)\frac{\partial k}{\partial p_j}\right] \tag{10}$$

where p_j is the structural parameter respect to which the partial derivative is computed and j is the layer sequential number [1].

The partial derivatives of the structural parameters dependent terms in (9) and (10) can be computed from the partial derivatives with respect to the structural parameters of eigenfunctions, phase and group velocity, and energy integral. The partial derivative of ε_0 e can be computed from the derivatives of the eigenfunctions

$$\frac{\partial}{\partial p_j}\varepsilon_0 = \frac{\partial}{\partial p_j}\frac{u^*(0)}{w(0)} \tag{11}$$

The partial derivative of $\chi(\Theta, \mathrm{h})$ can be obtained from the partial derivatives with respect to structural parameters of $A(h)$, $B(h)$ and $C(h)$, as given in [1]. The partial derivatives of phase and group velocity and energy integral are needed to compute the partial derivatives for k and A

$$\frac{1}{k}\frac{\partial k}{\partial p_j} = -\frac{1}{c}\frac{\partial c}{\partial p_j} \tag{12}$$

$$\frac{1}{A}\frac{\partial A}{\partial p_j} = -\left(\frac{1}{c}\frac{\partial c}{\partial p_j} + \frac{1}{u}\frac{\partial u}{\partial p_j}\frac{1}{I_1}\frac{\partial I_1}{\partial p_j}\right) \tag{13}$$

The partial derivative of phase velocity with respect to the structural parameters can be computed with the method described in [15]; the derivatives of group velocities can be computed with the asymptotic fast method developed in [1] that locally approximates the derivative of phase velocity using a cubic interpolation as shown in section 3. Following the formulations given in [12], [13] and [14], the evaluation of the partial derivatives of eigenfunctions $u(z)$, $w(z)$, $\sigma(z)$ and $\tau(z)$ is reduced to the determination of the partial derivatives of the layer constants A_m, B_m, C_m and D_m for the layers above the homogeneous half-space, and the constants A_n and B_n for the deepest structural unit.

We compute the derivatives of the elements of the (1x6) matrix that appear in the basic interface-matrix multiplication of Knopoff's method [13]:

$$\lfloor U^{m+1},\quad iV^{m+1},\quad W^{m+1},\quad R^{m+1},\quad iS^{m+1},\quad -U^{m+1}\rfloor \tag{14}$$

where U^i, V^i, W^i, R^i, S^i are the i-th interface elements in the fast form of Knopoff's method for Rayleigh-wave computation. In paper [1] the formalism is limited to the case of continental structures, where the first interface elements are

$$U^0 = -\gamma_1(\gamma_1 - 1), \qquad V^0 = 0, \qquad W^0 = (\gamma_1 - 1)^2, \qquad R^0 = \gamma_1^2, \qquad S^0 = 0 \tag{15}$$

with

$$\gamma_1 = 2\beta_1^2/\mathrm{c}^2 \tag{16}$$

When considering oceanic models, i.e. structural models with an uppermost liquid layer, equation (12) is no longer valid. The computation of differential seismograms in presence of an uppermost water layer needs a different formalism.

2. Case of oceanic structures

2.1. *The formalism*

For an oceanic model, the vanishing of the stress at the free liquid surface, combined with the continuity of displacement and stresses and the vanishing of the tangential component of the stress at the liquid-solid interface yields for the first interface element S^0 [11]

$$S^0 = \varrho_0 \tan P_0/\varrho_1 r_{\alpha 0}$$

where

$$\frac{r_{ai}}{\alpha} = \begin{cases} \sqrt{c^2/\alpha_i^2 - 1} & \text{if } c > \alpha_i \\ -i\sqrt{1 - c^2/\alpha_i^2} & \text{if } c < \alpha_i \end{cases} \tag{18}$$

$$P_0 = k r_{\alpha 0} d_0 \tag{19}$$

The presence of an uppermost liquid layer affects the expression for the energy integral that is required in multi-mode synthesis of seismograms. For a sequence of homogeneous layers, this integral can be written as

$$\mathrm{I} = \begin{cases} c^2\{[r_{\alpha 1}B_1]-[D_1]\}^{-2}\sum_{m=1}^{n} I_m & \text{for a continental structure} \\ c^2\{[r_{\alpha 1}B_1]-[D_1]\}^{-2}\sum_{m=0}^{n} I_m & \text{for an oceanic structure} \end{cases} \tag{20}$$

where

$$I_0 = \frac{\varrho_0 [r_{\alpha 0}B_0]^2}{2\omega c r_{\alpha 0}}\left[\sin P_0 \cos P_0 \left(1-1/r_{\alpha 0}^2\right) + P_0 \left(1+1/r_{\alpha 0}^2\right)\right] \tag{21}$$

At this point the partial derivatives of the first interface elements U^i, V^i, W^i, R^i, S^i can be easily computed from

$$\frac{\partial \gamma_1}{\partial \beta_j} = -\frac{4\beta_1^2}{c^3}\frac{\partial c}{\partial \beta_j} \qquad \text{(when j}\neq 1\text{)}$$

$$\frac{\partial \gamma_1}{\partial \beta_j} = \frac{4\beta_1}{c^2} - \frac{4\beta_1^2}{c^3}\frac{\partial c}{\partial \beta_j} \qquad \text{(when j=1)} \tag{22}$$

$$\frac{\partial \gamma_1}{\partial \alpha_j} = -\frac{4\beta_1^2}{c^3}\frac{\partial c}{\partial \alpha_j} \tag{23}$$

$$\frac{\partial \gamma_1}{\partial \varrho_j} = -\frac{4\beta_1^2}{c^3}\frac{\partial c}{\partial \varrho_j} \tag{24}$$

$$\frac{\partial}{\partial \beta_j} P_0 = -d_0 \frac{\omega_c}{c}\frac{\partial c}{\partial \beta_j} r_{\alpha 0} + d_0 \frac{\omega_c}{\alpha_0^2}\frac{\partial c}{\partial \beta_j}\frac{1}{r_{\alpha 0}} \tag{25}$$

$$\frac{\partial}{\partial \alpha_j} P_0 = \begin{cases} -d_0 \frac{\omega_c}{c}\frac{\partial c}{\partial \beta_j} r_{\alpha 0} + d_0 \frac{\omega_c}{\alpha_0^2}\frac{\partial c}{\partial \beta_j}\frac{1}{r_{\alpha 0}} & (\mathrm{j} \neq \mathrm{m}) \\ -d_0 \frac{\omega_c}{c}\frac{\partial c}{\partial \beta_j} r_{\alpha 0} + d_0 \frac{\omega_c}{\alpha_0^3}\left(\frac{\partial c}{\partial \beta_j}\alpha_0 - c\right)\frac{1}{r_{\alpha 0}} & (\mathrm{j} = \mathrm{m}) \end{cases} \tag{26}$$

$$\frac{\partial}{\partial \varrho_j} P_0 = -d_0 \frac{\omega_c}{c}\frac{\partial c}{\partial \beta_j} r_{\alpha 0} + d_0 \frac{\omega_c}{\alpha_0^2}\frac{\partial c}{\partial \beta_j}\frac{1}{r_{\alpha 0}}$$

The other derivatives needed to compute partial derivatives of eigenfunctions and energy integrals can be found in [1].

2.2. *Test on partial derivatives and differential seismograms*

We compute the partial derivatives and the differential seismograms using two oceanic structural models; one with a 1km-thick uppermost water layer and the other with a 4km-thick water layer. We compare the results of our analytical calculations with those obtained through numerical differentiation, to study the effect of neglecting the term (17) in the computation of partial derivatives and synthetic differential seismograms.

We consider, for the solid part, the structural model reported in Fig. 1, where the upper 250 km of the structural model are plotted. To compute synthetic and differential seismograms we consider a source located at the depth of 33 km and a double-couple mechanism (δ=37°, λ=283°, azimuth of the station with respect to the fault strike =260°). The seismograms have been scaled with a moment of 6.5×10^{19} Nm; they are all computed for a distance of 1000 km from the source and an upper frequency limit of 0.1Hz.

We compute the differential seismograms with respect to the change of shear velocity in each layer using a first-order centred numerical differentiation according to [1]. The adopted differentiation formula is

$$\frac{\partial s\lfloor t, p_j(z)\rfloor}{\partial p_j} = \frac{s\lfloor t, p_j(z)+\delta p_j(z)\rfloor - \lfloor t, p_j(z) - \delta p_j(z)\rfloor}{2\delta p_j(z)} \tag{27}$$

where $\delta p_j(z) = 0.005$ kms^{-1} is the shear-wave velocity perturbation.

In Fig. 2 and 3 the differential seismograms computed analytically are plotted together with those computed numerically, for the models with 1km and 4 km of

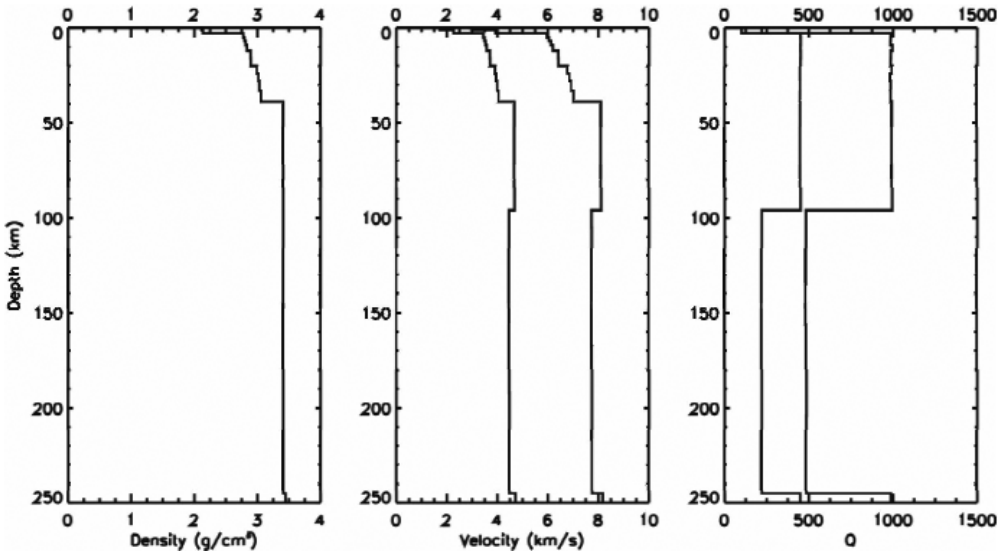

Fig. 1. Structural model (upper 250 km) used to compute the synthetic and differential seismograms.

water, respectively. We show the results for six structural layers (labelled 2, 8, 12, 14, 20, 24).

The solid lines correspond to the analytical calculations, whereas the dashed lines correspond to the numerical differentiation.

To show the effect of neglecting the derivative of the term (17) we consider the partial derivatives of the eigenfunction u, computed for the fundamental and the first higher mode, for the models with a 1km- and 4km-thick liquid layer respectively. In Fig. 4 the dotted and dashed lines correspond to the numerical calculation and the analytical calculation made with the new code that takes into account the derivatives of equation (17). The dot-dashed lines represent the partial derivatives computed analytically, but neglecting the presence of the water layer. The presence of a surface liquid layer severely affects the computation of partial derivatives. The effect is dramatically evident in the case of a 4km-thick water layer.

The effect on differential seismograms of these differences in partial derivatives is the introduction of noise, as we can see in Fig. 5. In this picture the synthetic differential seismograms computed with respect to shear-wave velocity for layer 2 are reported.

The upper trace corresponds to a structural model with 1km-thick water layer, the second one with a 4km-thick water layer.

The methodology proposed in [1] to compute synthetic differential seismograms has been used in waveform inversions [2], where a set of seismograms is inverted to estimate the structural parameters. This formalism, that handles only

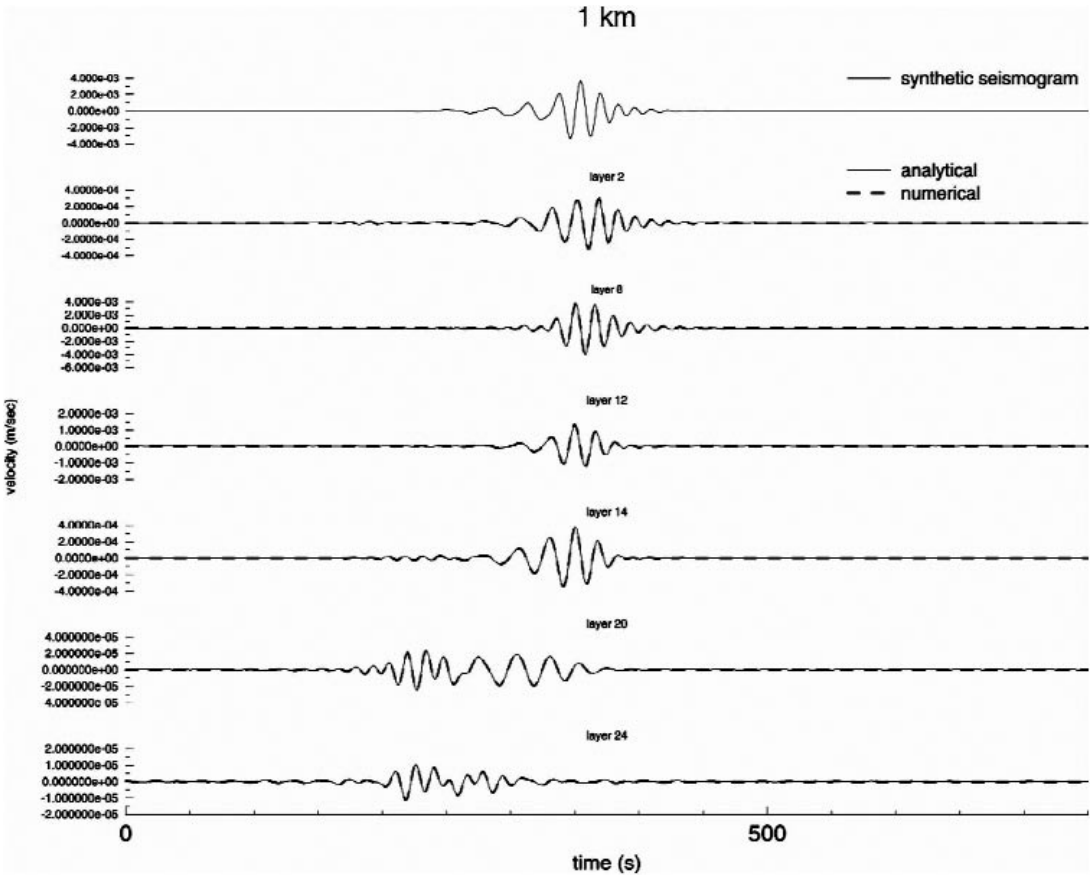

Fig. 2. Seismograms (first trace) and differential seismograms (remaining traces) computed with respect to shear wave velocity for the layers indicated upon each trace. The solid lines correspond to differential seismograms computed analytically, dashed lines to those computed numerically. The computation was performed using a structural model with a 1km-thick liquid layer.

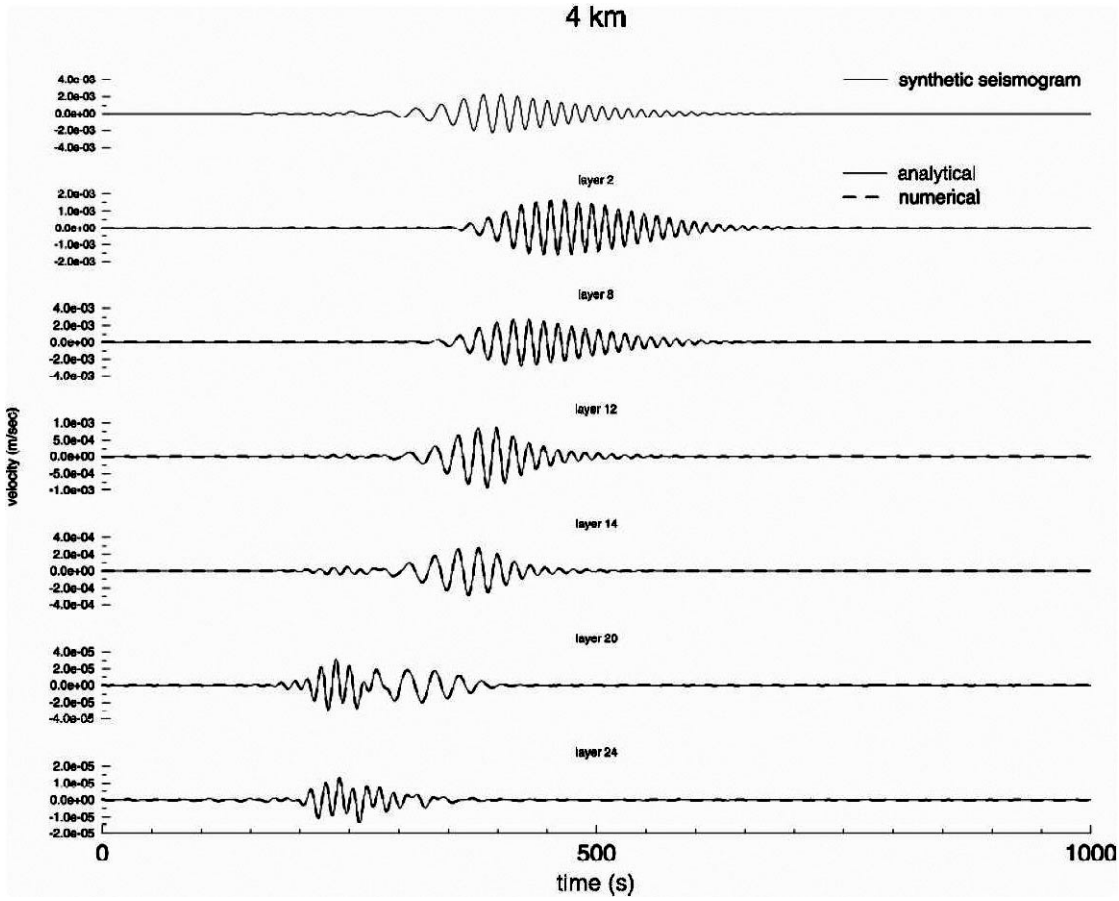

Fig. 3. Seismograms (first trace) and differential seismograms (remaining traces) computed with respect to shear wave velocity for the layers indicated upon each trace. The solid lines correspond to differential seismograms computed analytically, dashed lines to those computed numerically. The computation was performed using a structural model with a 4km-thick liquid layer.

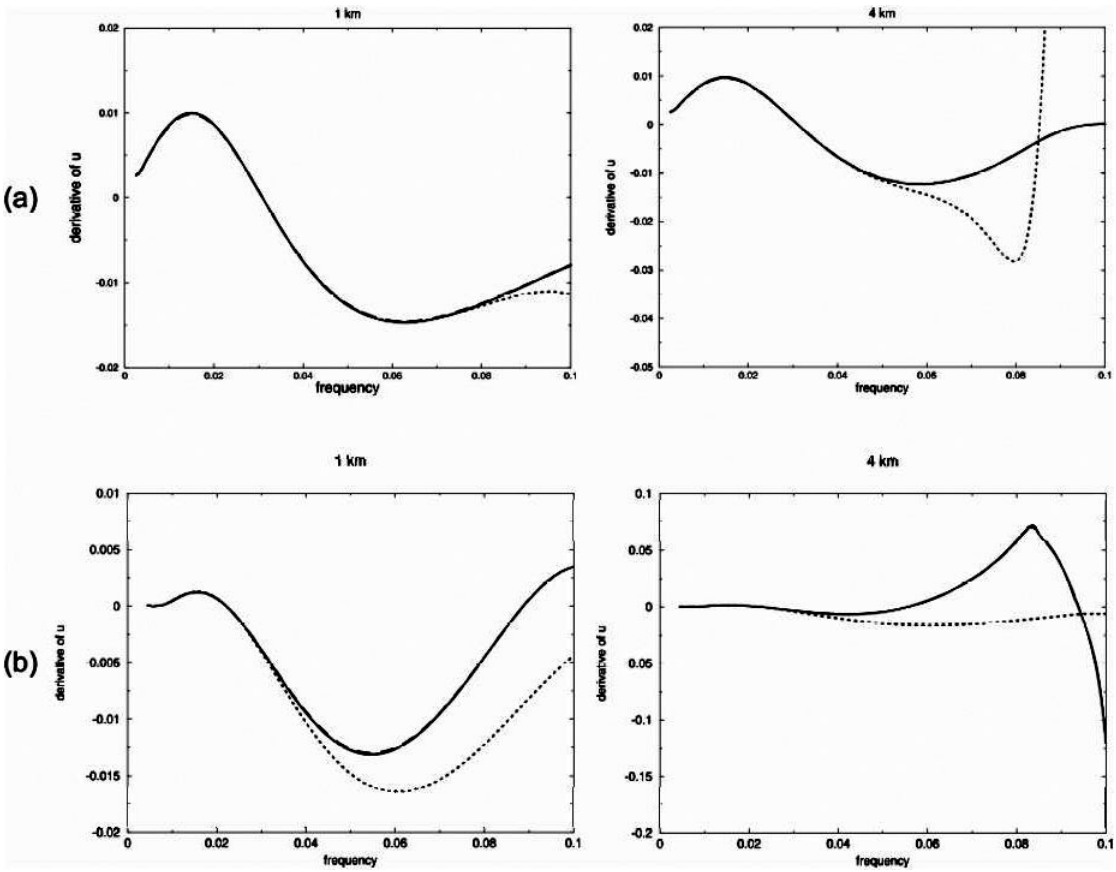

Fig. 4. Partial derivatives of eigenfunction u with respect to layer 2. The solid lines correspond to the partial derivatives computed analytically while the dashed lines to those computed numerically. The dotted lines are the partial derivatives calculated analytically neglecting the formalism for oceanic models. Left: with 1km-thick liquid layer; right: with 4km-thick liquid layer; (a) fundamental mode; (b) first higher mode.

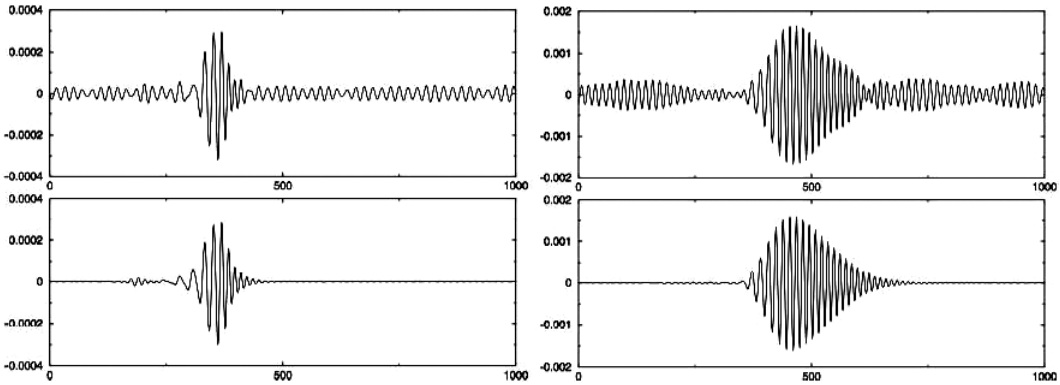

Fig. 5. Synthetic differential seismograms with respect to shear wave velocity of layer 2 using partial derivative obtained analytically neglecting the formalism for oceanic models (upper trace) and with the formalism for oceanic models (lower trace). Left: with 1km-thick liquid layer; right: with 4km-thick liquid layer.

continental structural models, can be applied, in general, only for very low frequencies, as we can see from figure 4 and figure 5. At high frequencies, for oceanic models the new formalism has to be applied in the calculation of partial derivatives. When dealing with high frequencies the following additional extension of [1] is necessary.

3. Computation of partial derivatives of group velocity

To compute partial derivatives of group velocity with respect to structural model parameters [1] suggest a fast asymptotic method. The group velocity, u, is equal to the partial derivative of the frequency, ω, with respect to the wave number, k:

$$u = \left.\frac{\partial\omega}{\partial k}\right|_{p_j} = \frac{c}{1 - \frac{\omega}{c}\left.\frac{\partial c}{\partial\omega}\right|_{p_j}} . \tag{28}$$

Using the implicit function theory, the partial derivative of group velocity with respect to the model parameters p_j ($p_j=\beta_j$, α_j, ϱ_j) can be written as

$$\left.\frac{\partial u}{\partial p_j}\right|_{\omega} = \frac{u}{c}\left(2 - \frac{u}{c}\right)\left.\frac{\partial c}{\partial p_j}\right|_{\omega} + \omega\,\frac{u^2}{c^2}\,\frac{\partial}{\partial\omega}\left(\left.\frac{\partial c}{\partial p_j}\right|_{\omega}\right)\Bigg|_{p_j}, \tag{29}$$

where the calculation of the partial derivative for the phase velocity derivative with respect to frequency,

$$\frac{\partial}{\partial\omega}\left(\frac{\partial c}{\partial p_j}\bigg|_{\omega}\right)\bigg|_{p_j} \tag{30}$$

is computationally demanding. The paper [11] suggested a numerical approach to obtain this derivative. Improving their method, authors of paper [1] compute it analytically as follows. Considering as structural model parameters the S-wave velocities, β_j, for a given Rayleigh wave mode the expression of $(\partial c/\partial\beta_j)|_{\omega}$ [5] is

$$\frac{\partial c}{\partial\beta_j}\bigg|_{\omega} = \frac{\beta_j\varrho_j}{uI_1}\left[\left(y_1 + \frac{1}{k}\frac{dy_2}{dz}\right)^2 + \frac{4}{k}\frac{dy_1}{dz}y_2\right] \tag{31}$$

where $y_1=u(z)/w(0)$, $y_2=w(z)/w(0)$. The eigenfunctions can be represented through a linear combination of exponential functions [5], which, at a given frequency, ω, can be written as

$$\exp\left[\pm i\frac{\omega}{c}d_m r_{\beta m}\right]. \tag{32}$$

Therefore, $(\partial c/\partial\beta_j)|_{\omega}$ in eq. (29) is a linear combination of exponential functions. The exponential function in (32) can be approximated through a series expansion, which may correspond to a low-order polynomial when the argument is small.

In the calculations suggested in [1], for each mode the functions $(\partial c/\partial\beta_j)|_{\omega}$ are defined for a discrete number of frequency points, ω_l ($l = 1, 2, \ldots, N$), and they are locally approximated using a cubic spline polynomial:

$$\frac{\partial c}{\partial\beta_j}\bigg|_{\omega} = a_l\omega^3 + b_l\omega^2 + c_l\omega + d_l \tag{33}$$

where the coefficients a_l, b_l, c_l and d_l are determined from $(\partial c/\partial\beta_j)|_{\omega}$ at each frequency, ω_l, using the two adjacent frequency values (i.e. ω_{l-1} and ω_{l+1}), by imposing the smoothness of the first derivative and the continuity of the second derivative, both within the interval and its endpoints [10]. To constrain the interpolation properly, at the two end frequency points of each mode, the method developed in [11] is enforced.

Using this method it is possible to compute the partial derivatives of group velocity, with respect to the structural parameter of each layer, starting from the partial derivatives of phase velocity in an analytic way, limiting the numerical computations at only two frequency points for each mode.

The algorithm gives good results if we consider long periods but it is not satisfying when it is applied to high frequencies. The reason is that for high frequen-

cies (above 0.1 Hz) the functions $(\partial c/\partial \beta_j)|_\omega$ related to higher modes can present rapid gradient changes and if this function is interpolated with a polynomial, as described in [10], pronounced oscillations appear in correspondence of these "discontinuity" points (with respect to the discretization step used in the computations of spectral properties, like e.g. phase velocities). As example, in Fig. 7, 8 and 9, are shown partial derivatives of phase and group velocity for different modes with respect to Vs of the fourth layer for the model shown in Fig. 6. The partial derivatives are computed using a maximum frequency of 1 Hz, with a sampling step of 0.005 Hz. For the fundamental mode the partial derivative of phase velocity is a continuous function and can be locally approximated by a polynomial. For the first higher mode and for frequencies above 0.1 Hz the functions $(\partial c/\partial \beta_j)|_\omega$ present some discontinuity points and the computation of the partial derivatives of group velocity with the method developed in [1] fails in proximity of these points. The problem arises every time a function $c'(\omega) = (\partial c/\partial \beta_j)|_\omega$ presents a discontinuity in its first derivative, i.e., being phase velocity computed at a set of discrete points, the problem may arise every time the quantity

$$\left|\frac{c'(\omega_{i+1})-c'(\omega_i)}{\Delta\omega} - \frac{c'(\omega_i)-c'(\omega_{i-1})}{\Delta\omega}\right| \frac{1}{\Delta\omega} = \frac{\left|c'(\omega_{i-1})+c'(\omega_{i+1})-2c'(\omega_i)\right|}{\Delta\omega^2} \tag{34}$$

overcomes a certain threshold.

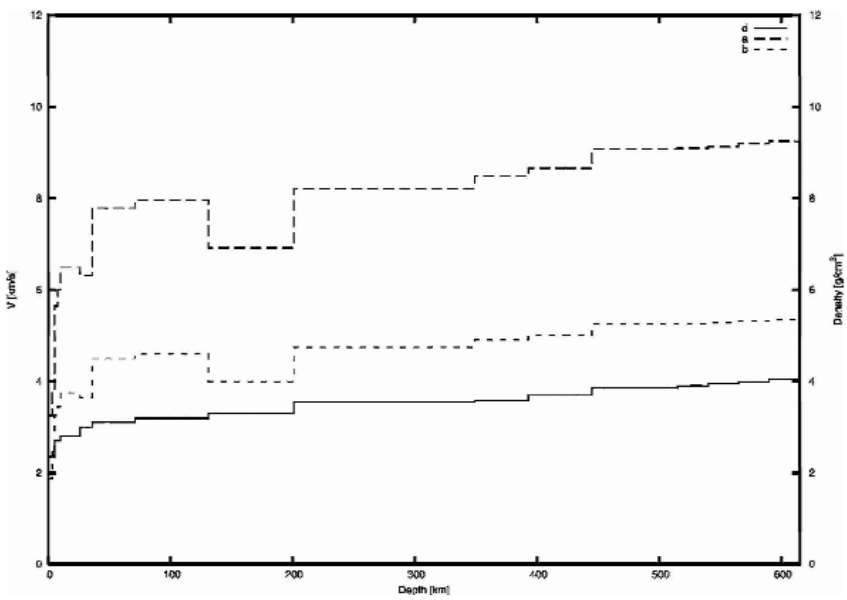

Fig. 6. Structural model used to test the modified code.

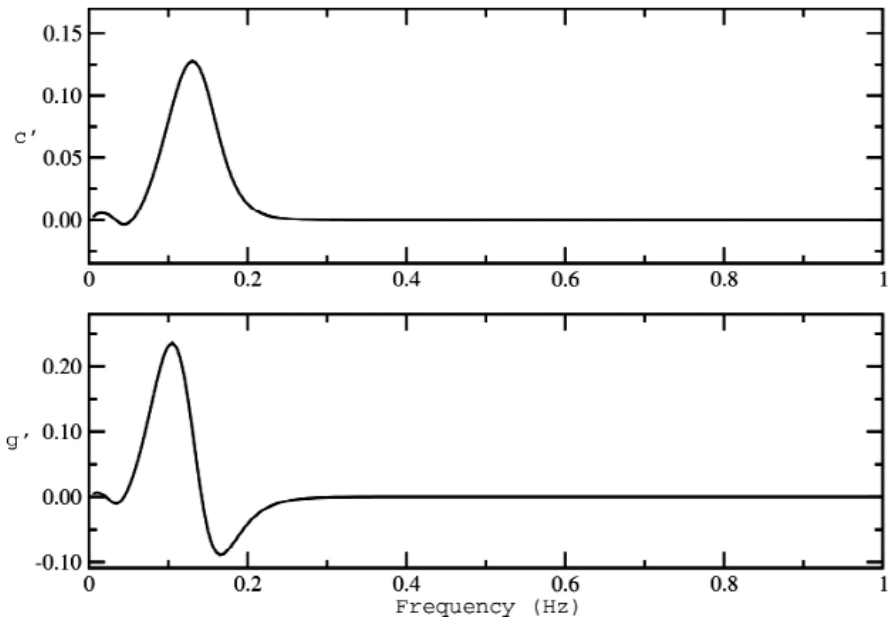

Fig. 7. a) (Top) Partial derivative of phase velocity of fundamental mode with respect to Vs of the fourth layer. b) (Bottom) Partial derivative of group velocity computed interpolating the function in Fig. 7a with a polynomial as described in [10].

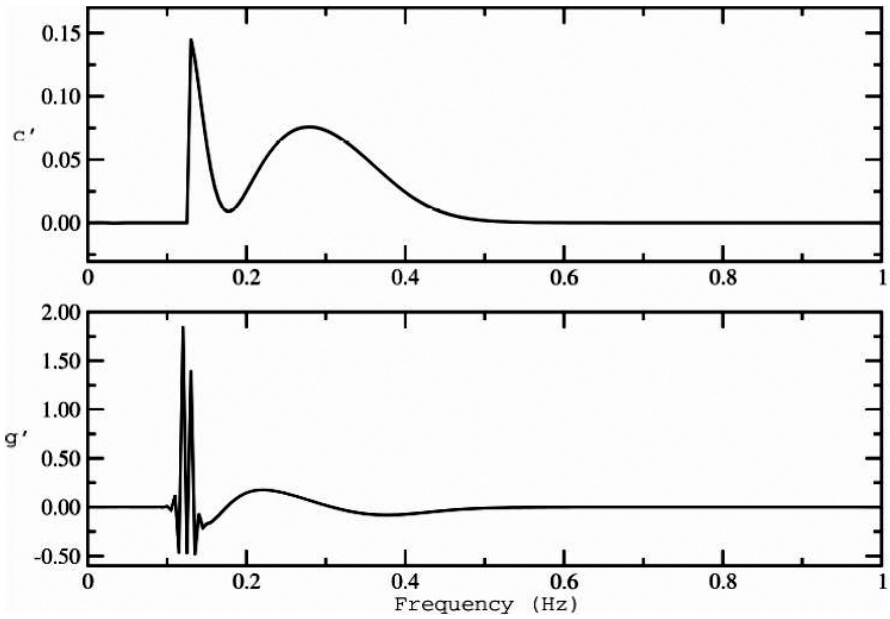

Fig. 8. Same as Fig. 7, but for the first higher mode.

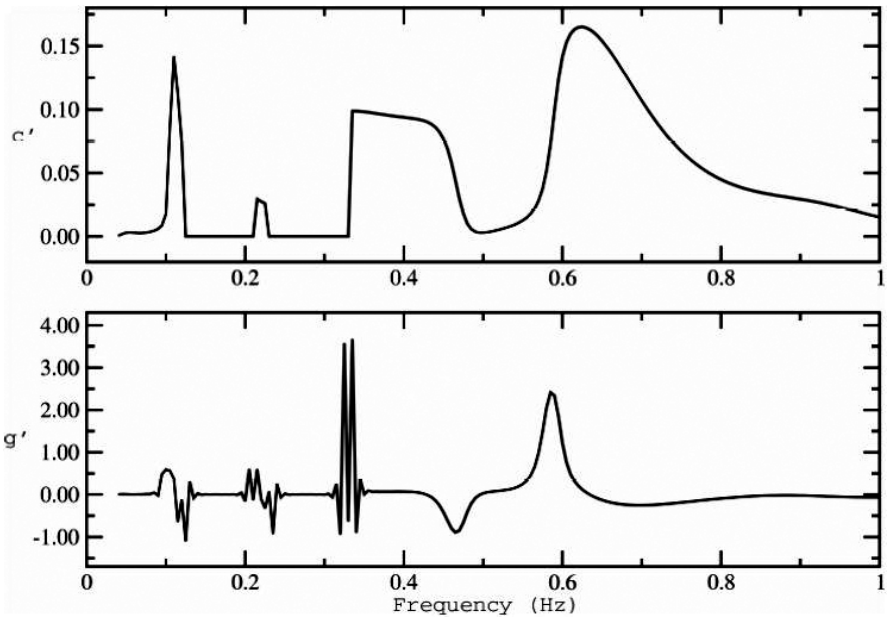

Fig. 9. Same as Fig.7, but for the fourth higher mode.

To eliminate, or better to reduce this problem below the numerical noise level, without using the numerical method [11] for all the frequencies ω_i, the code for the computation of partial derivatives of group velocity has been modified. If the first derivatives of the function $(\partial c/\partial \beta_j)|_\omega$ present n discontinuity points ω_k (k=1,…, n), where ω_0 and ω_n are the two end frequencies, we can split the whole domain into n-1 smaller intervals delimited by $[\omega_k, \omega_{k+1}]$ (k = 1, …, n-1). In each of these intervals the function $(\partial c/\partial \beta_j)|_\omega$ has continuous first derivative and so we can apply the method developed by [1]. With this procedure most of the values of group velocity partial derivatives are computed in an analytical way, leaving the numerical computation to a limited number of points. Fig. 10 shows the partial derivatives of group velocity calculated with the modified code. The results have been tested comparing them with the partial derivative of group velocity with respect to structural parameter computed with the numerical method [11] (Fig 11). With these modifications, the partial derivatives can be computed over a wide range of frequencies, therefore they can be used for different kinds of applications.

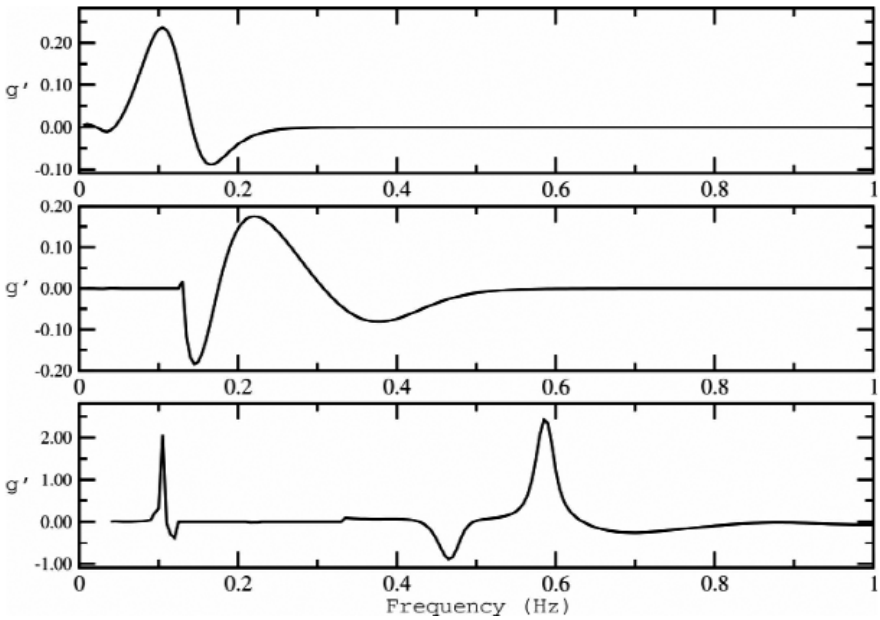

Fig. 10. Partial derivatives of group velocity with respect to Vs of the fourth layer computed using the modified version of the method described in [1].

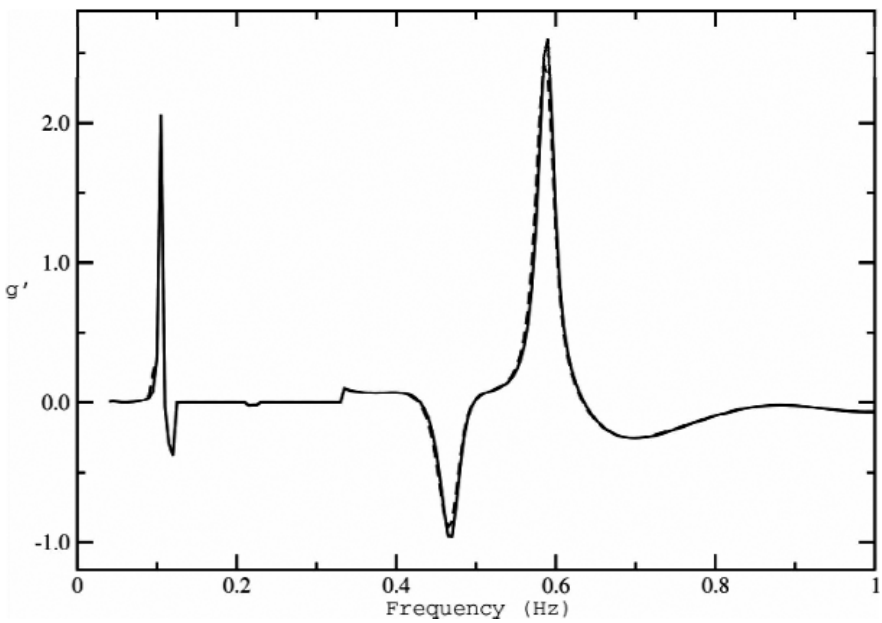

Fig. 11. Comparison between partial derivative of group velocity for the fourth higher mode with respect to Vs of the fourth layer, computed using the modified version of the method described in [1] (solid line) and the numerical method [11] (dotted line).

4. Conclusions

A fast and accurate method for the computation of differential seismograms with respect to structural model parameters has been proposed in [1]. The original methodology was developed for continental structures and can be applied in general for low frequencies only. We have extended the existing formalism and the related computer codes to evaluate: (1) differential seismograms in case of oceanic structural models with an uppermost liquid layer, and (2) partial derivatives of group velocity for frequencies higher than 0.05Hz. In this paper we present the formalism used for the analytical calculation and the comparison of the results of our analytical calculations with those obtained through numerical differentiation.

With our improvements, the methodology can be used in waveform inversions for structural parameters in different environments and for different ranges of frequencies.

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