

Ray tracing on a heterogeneous sphere by Lie series

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SUMMARY

We propose a method for fast analytical ray tracing on a heterogeneous sphere for surface waves. We first select the specific coordinates of orbital motion which have action/angle properties. We then apply the Lie perturbation approach and, when the square of the slowness is expanded in spherical harmonics, we obtain an analytical formula for the perturbed parameters of the ray. These expressions are sensitive to both the odd and even parts of the expansion. Traveltimes are computed by perturbation, while geometrical spreading is estimated numerically between two nearby perturbed rays. For the ‘Gulf of Alaska’ earthquake of November 1987, the analytical ray follows the same deviations with respect to the great circle as the numerical one, when we use the phase velocity model of Montagner & Tanimoto (1990) at period of 167 s. The agreement is excellent for traveltimes computations. When the numerical ray tracing predicts a focus/defocusing effect, the perturbed ray tracing gives the same trend. Moreover, variations of the shooting angles between trains can be as high as 20° which might modify the radiation pattern seen by the station for different trains. When the perturbed ray deviates too strongly, a reinitialization technique will guarantee a given accuracy. This reinitialization, which is not required for long periods (>150 s), is probably necessary at shorter periods.

Key words: Alaska earthquake, Lie series perturbation, ray tracing, surface waves.

1 INTRODUCTION

Extracting information on laterally varying Earth structure from surface-wave seismograms requires fast methods which simplify the forward problem to a satisfactory level for inversion. Simple assumptions, as the great circle path approximation used in seismic tomography, already give interesting global pictures of the Earth’s upper mantle (Nakanishi & Anderson 1984; Nataf, Nakanishi & Anderson 1984, 1986; Tanimoto & Anderson 1985; Montagner & Tanimoto 1990). Using lateral variations only along the major and minor great circle paths also leads to seismogram inversion (Woodhouse & Dziewonski 1984; Tanimoto 1984, 1987b, 1988). Further improvements, such as the use of Gaussian beam methods, have been undertaken (Yomogida & Aki 1987), but much work remains to be done to improve the resolution of the mantle structure. More elaborate methods are available [see references in Park & Gilbert (1986) or in Lognonné & Romanowicz (1990)] for synthesizing seismograms, but a compromise between complexity of the underlying theory and computer speed has to be made. Taking into account the small amplitude of lateral heterogeneities in the upper mantle for the long-period range of surface waves, one might hope that perturbation techniques will apply to this problem. Some simplifications, for computing the phase as well as the amplitude, have been proposed by Woodhouse & Wong (1986) for the ray method and by Romanowicz (1987) for the normal modes formulation. These formulations, which are equivalent to first order, require the additional knowledge of first and second derivatives of velocity perpendicular to the great circle path. It is not yet clear how adequate these approximations are and whether we need further improvements, provided by more complete perturbation formulations (Tsuboi, Geller & Morris 1985; Park 1987; Snieder & Romanowicz 1988; Lognonné & Romanowicz 1990) to progress with the inverse problem.

We propose a theory based on recent Lie series perturbation techniques in order to evaluate the ray analytically at the station position when lateral heterogeneities are involved. The perturbation technique is similar to the one of Woodhouse & Wong (1986) but we apply it to very specific variables obtained by a canonical transformation introduced in seismology by Dahlen & Henson (1985) and Henson & Dahlen (1986). We extend and complete the work of Virieux (1989). These techniques have recently been applied in the problem of oceanographic tomography (Miller 1986; Wunsch 1987). Because the

Lie series perturbation technique is not familiar to most seismologists, we shall present the method of ray tracing at a given frequency in this paper. Constructing a complete seismogram will be the purpose of future work.

We shall assume that the seismograms are sensitive only to lateral heterogeneities of the Earth. Corrections for ellipticity as well as for the rotation of the Earth (Dahlen 1975; Woodhouse & Dziewonski 1984) are perturbations which do not interact with perturbations of lateral heterogeneities. In a more complete analysis, we might have taken into account these effects of rotation (Backus 1962), as well as these effects of ellipticity (Jobert 1976; Mochizuki 1989) in the ray tracing system itself.

The Lie series perturbation method applies in a very elegant way to problems cast into an Hamiltonian formulation, which we introduce now.

2 THE HAMILTONIAN APPROACH

Because we are going to exploit the Hamiltonian structure of ray tracing, we must describe how we define the Hamiltonian. In order to do so, we start from the high-frequency approximation which allows one to represent a scalar surface displacement field by the following expression:

$$d(\mathbf{x}, t) = A(\mathbf{x}, t)e^{i\psi(\mathbf{x}, t)}, \quad (1)$$

where \mathbf{x} is the position on the involved surface and t is time. A is the slowly varying amplitude and ψ is the rapidly varying phase. Let us introduce a local wave vector and a local instantaneous frequency by

$$\mathbf{k} = \nabla\psi, \quad \omega = -\frac{\partial\psi}{\partial t}, \quad (2)$$

where ∇ is the surface nabla operator. One can find an eikonal equation which can be expressed as a local dispersion relation (Woodhouse 1974; Jobert & Jobert 1987) $\omega = \omega(\mathbf{x}, \mathbf{k})$. Taking into account the definitions of \mathbf{k} and ω (equation 2), this equation leads to a Hamilton–Jacobi equation for $\psi(\mathbf{x}, t)$:

$$\frac{\partial\psi}{\partial t} + \omega(\nabla\psi, \mathbf{x}) = 0, \quad (3)$$

from which one can deduce the Hamilton's canonical equations:

$$\dot{\mathbf{x}} = \nabla_{\mathbf{k}}\omega, \quad \dot{\mathbf{k}} = -\nabla_{\mathbf{x}}\omega, \quad (4)$$

where dots denote the time derivative. Since ω has no explicit dependence upon time, we also have $\dot{\omega} = 0$. The variational problem associated with the Hamiltonian, ω , is given by $\delta\psi = 0$, stating that the phase is stationary along the ray path (Landau & Lifchitz 1969). These equations are very general and are valid for any anisotropic medium. Let us turn our attention to the isotropic case. Defining the wavenumber by

$$k = \sqrt{k^\beta k_\beta} = \sqrt{g^{\alpha\beta} k_\alpha k_\beta}, \quad (5)$$

where $g^{\alpha\beta}$ is the contravariant metric tensor of the coordinate system we use, the local dispersion relation can be written

$$\omega(k_\sigma, x^\sigma) = \omega(k, x^\sigma). \quad (6)$$

This expression is also valid for transversely isotropic media because ω is azimuthally independent (Tanimoto 1987a). We invert equation (6) and write k with respect to ω and x^σ as the local dispersion relation:

$$k = k(\omega, x^\sigma). \quad (7)$$

One can deduce the following equations:

$$\frac{dx^\sigma}{dt} = \frac{1}{k} \frac{\partial\omega}{\partial k} g^{\sigma\nu} k_\nu, \quad \frac{dk_\sigma}{dt} = -\frac{\partial\omega}{\partial x^\sigma} - \frac{1}{2k} \frac{\partial\omega}{\partial k} \frac{\partial g^{\alpha\beta}}{\partial x^\sigma} k_\alpha k_\beta. \quad (8)$$

Let us introduce the group velocity $U = \partial\omega/\partial k$, as well as the phase velocity $c = \omega/k$. The sampling parameter t along the ray can be converted to the arclength s by $U ds = dt$. This choice modifies the Hamiltonian and one can write the canonical equations as

$$\frac{dx^\sigma}{ds} = \frac{1}{k} g^{\sigma\nu} k_\nu = \frac{1}{k} k^\sigma, \quad \frac{dk_\sigma}{ds} = \left(\frac{\partial k}{\partial x^\sigma} \right)_\omega - \frac{1}{2k} \frac{\partial g^{\alpha\beta}}{\partial x^\sigma} k_\alpha k_\beta, \quad (9)$$

where k^σ are the contravariant components of the wave vector defined by $k^\sigma = g^{\sigma\nu} k_\nu$. These equations show explicitly that rays are independent of the group velocity, and they can be obtained from the variational problem (where the phase traveltime

along the ray path is stationary) for $x^\sigma(s)$:

$$\delta \int k(\omega, x^\sigma) ds = 0 \quad (10)$$

subject to the constraint

$$g_{\sigma\nu} \frac{dx^\sigma}{ds} \frac{dx^\nu}{ds} = 1. \quad (11)$$

These equations can also be derived from the Hamiltonian given by

$$H(k_\sigma, x^\sigma) = \sqrt{g^{\alpha\beta} k_\alpha k_\beta} - k(\omega, x^\sigma) = 0. \quad (12)$$

Up to now, we have simply reproduced standard results (Woodhouse & Wong 1986; Keilis-Borok 1989). Introducing now another variable ζ instead of the arclength s by $ds = k d\zeta$, we can write the Hamilton's canonical equations in a more simple form:

$$\begin{aligned} \frac{dx^\sigma}{d\zeta} &= k^\sigma, \\ \frac{dk_\sigma}{d\zeta} &= \frac{1}{2} \left(\frac{\partial k^2}{\partial x^\sigma} \right)_\omega - \frac{1}{2} \frac{\partial g^{\alpha\beta}}{\partial x^\sigma} k_\alpha k_\beta. \end{aligned} \quad (13)$$

These equations may be obtained from the variational problem (saying also that the phase traveltime along the ray path is stationary) for $x^\sigma(\zeta)$:

$$\delta \int k^2(\omega, x^\sigma) d\zeta = 0, \quad (14)$$

or derived from the Hamiltonian given by

$$H(k_\sigma, x^\sigma) = \frac{1}{2} [g^{\alpha\beta} k_\alpha k_\beta - k^2(\omega, x^\sigma)] = 0. \quad (15)$$

These three Hamiltonians [given by equations (3), (12) and (15) and the three associated variational problems] lead to the same trajectories or rays as shown by Dubrovine, Novikov & Fomenko (1982, p. 311). Let us emphasize that the different variational problems have somewhat different constraints. The first one, $\delta\psi = 0$, implies a constant time t , the second one, equation (9), a constant length s and the third, equation (13), gives a constant parameter ζ . The choice between them will depend on the problem at hand. The first formulation would be well-suited because the time is obtained directly, but the presence of the group velocity makes the equations difficult to solve (Tanimoto 1987a). The second formulation is the most frequently used approach in surface-wave ray tracing, because one does not require the group velocity in the ray tracing equations. Moreover, the ray tracing equations are identical to the non-dispersive body-wave ray tracing (Aki & Richards 1980), allowing the use of body-wave ray tracing numerical codes. The group velocity is only involved for computing the time, which is now done separately. The third formulation has received increasing interest in body-wave approach (Burridge 1976) because it gives the simplest form for the equations. It also introduces a formal equivalence between a ray and a particle trajectory and allows us to construct solutions borrowed from celestial mechanics results (Henson & Dahlen 1986; Virieux 1989). The variable ζ has now a physical meaning: the quantity ζ/ω is the time connected with the associated particle motion (Goldstein 1980, p. 484).

Many other Hamiltonians can be introduced. In body-wave ray tracing, for example, one can reduce the number of variables with the relation $H = 0$. This relation, of course, can also be used to check accuracy of the ray tracing. It turns out that the reduced Hamiltonian is too complex for our purpose. Consequently, the zero value of the Hamiltonian is not used further and any constant might be taken. Once initial conditions define this constant, the Hamiltonian stays at this value along rays. We shall note this constant as E from the analogy with the constant energy of an isolated system. However, the geometrical interpretation of E is the unicity of the hypersurface in the phase space where rays are. Reduced Hamiltonians define this hypersurface as the phase space itself. Investigations around this hypersurface are important for ray tracing perturbations.

We now turn to a more specific set of coordinates—angles θ and ϕ (Fig. 1)—for surface-wave ray tracing. Introducing the slowness $u(\theta, \phi)$, by the following definitions: $k^2(\omega, \theta, \phi) = \omega^2/c^2(\theta, \phi) = \omega^2 u^2(\theta, \phi)$ and the new vector \mathbf{p} by $\mathbf{k} = \omega \mathbf{p}$, we obtain the following Hamiltonian:

$$H(\theta, \phi, p_\theta, p_\phi) = \frac{1}{2} \left(\frac{p_\theta^2}{a^2} + \frac{p_\phi^2}{a^2 \sin^2 \theta} - u^2(\theta, \phi) \right) = E, \quad (16)$$

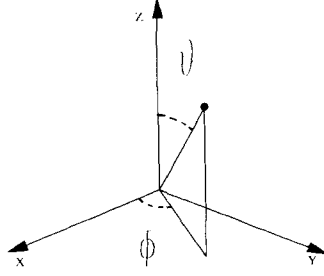


Figure 1. Spherical coordinates used for ray tracing equations.

with the implicit sampling parameter τ , defined by ζ/ω and where a is the radius of the Earth. The canonical equations will be

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial H}{\partial p_\theta}, \quad \frac{\partial p_\theta}{\partial \tau} = -\frac{\partial H}{\partial \theta}, \quad \frac{\partial \phi}{\partial \tau} = \frac{\partial H}{\partial p_\phi}, \quad \frac{\partial p_\phi}{\partial \tau} = -\frac{\partial H}{\partial \phi}. \quad (17)$$

This Hamiltonian is very similar to the one used by Backus (1962) for studying the effect of the rotation of the Earth on surface waves. The Hamiltonian defined by Woodhouse & Wong (1986) is for comparison:

$$\sqrt{\frac{p_\theta^2}{a^2} + \frac{p_\phi^2}{a^2 \sin^2 \theta}} - u(\theta, \phi) = 0. \quad (18)$$

Introducing the travelttime of a harmonic wave by $\psi = \omega T$, we find $\mathbf{p} = \nabla \mathbf{T}$, which allows us to rewrite the relation (15) under the usual form for an eikonal:

$$\frac{1}{a^2} \left(\frac{\partial T}{\partial \theta} \right)^2 + \frac{1}{a^2 \sin^2 \theta} \left(\frac{\partial T}{\partial \phi} \right)^2 = u^2(\theta, \phi). \quad (19)$$

The square of slowness arises as the natural quantity describing the lateral heterogeneity of the Earth (Červený 1987; Virieux, Farra & Madariaga 1988), and we always refer to this quantity from now on.

Let us construct exact solutions for a homogeneous sphere with the Hamiltonian defined by (16) and associated canonical equations (17).

3 THE ZERO-ORDER SOLUTION

Solving the ray tracing on a homogeneous sphere is simple and gives the great circle connecting the source and the station. Because we want to go one step further in the next section, we shall proceed in a more involved way by using canonical transformation methods, where the Hamiltonian approach shows its efficiency. We want to construct a transformation from variables $(\theta, \phi, p_\theta, p_\phi)$ to new variables $(\beta_1, \beta_2, J_1, J_2)$ that will make ray tracing (17) simpler to solve. This transformation may be constructed from a generating function $S(\tau, \theta, \phi, J_1, J_2)$ and the equations

$$p_\theta = \frac{\partial S}{\partial \theta}(\tau, \theta, \phi, J_1, J_2), \quad p_\phi = \frac{\partial S}{\partial \phi}(\tau, \theta, \phi, J_1, J_2), \quad (20a)$$

$$\beta_1 = \frac{\partial S}{\partial J_1}(\tau, \theta, \phi, J_1, J_2), \quad \beta_2 = \frac{\partial S}{\partial J_2}(\tau, \theta, \phi, J_1, J_2). \quad (20b)$$

We solve relations (20b) in order to get θ and ϕ with respect to $(\tau, \beta_1, \beta_2, J_1, J_2)$ and then insert these solutions into relations (20a) to get p_θ and p_ϕ with respect to $(\tau, \beta_1, \beta_2, J_1, J_2)$. In this formulation, the generating function S uses mixed coordinates. The transformed Hamiltonian is given by

$$K(\beta_1, \beta_2, J_1, J_2) = H(\theta, \phi, p_\theta, p_\phi) + \frac{\partial S}{\partial \tau}(\tau, \theta, \phi, J_1, J_2). \quad (21)$$

In order to obtain a canonical transformation, we select a canonical set as $(\beta_1, \beta_2, J_1, J_2)$ which guarantees the canonical equations:

$$\frac{\partial \beta_1}{\partial \tau} = \frac{\partial K}{\partial J_1}, \quad \frac{\partial J_1}{\partial \tau} = -\frac{\partial K}{\partial \beta_1}, \quad \frac{\partial \beta_2}{\partial \tau} = \frac{\partial K}{\partial J_2}, \quad \frac{\partial J_2}{\partial \tau} = -\frac{\partial K}{\partial \beta_2}. \quad (22)$$

Two choices give simple solutions. The transformed Hamiltonian may be independent of coordinates. In this case, the generating function is called the principal function or action. The variables β_1, β_2, J_1 and J_2 are constant. Another choice assumes

a Hamiltonian function of J_1 and J_2 only. The canonical equations (22) are solvable with J_1 and J_2 constant and β_1 and β_2 linear functions of τ . The associated generating function is now called the characteristic function. Because our Hamiltonian is τ -independent and is expressed only with J_1 and J_2 , it will also be constant. Consequently, it is possible to construct immediately a new generating function giving a Hamiltonian equal to zero. We simply have to subtract the term τK from the generating function. We are, therefore, back to the first choice which we shall consider in what follows.

The only systematic method for obtaining an analytical solution is additive separation of variables which is allowed by the specific structure of our selected Hamiltonian and widely used in celestial mechanics (Goldstein 1980). This is the *a posteriori* justification of the introduced τ parameter.

For a homogeneous sphere, we construct the solution using the systematic procedure of the Hamiltonian formulation in Appendix A. For a quicker way to obtain the solution, we refer the reader to Virieux (1989), as well as for the geometrical interpretation and the action/angle properties of the new quantities. Let us quote here only the final results. The solution, which is the great circle connecting the source and the station in this order, is given by the following expressions:

$$\cos \theta = \sin \Theta \sin (2\pi w_1), \quad p_\theta = \pm \frac{1}{2\pi} \sqrt{J_1^2 - \frac{J_2^2}{\sin^2 \theta}}, \quad \text{tg}(\phi - 2\pi w_2) = \cos \Theta \text{tg}(2\pi w_1), \quad p_\phi = \frac{J_2}{2\pi}, \quad (23)$$

where the appropriate sign is found from initial values. The variables w_1 and w_2 are defined respectively by $v_1\tau + \beta_1$ and $v_2\tau + \beta_2$. The parameters Θ and Φ are the coordinates of the pole associated with the great circle. They are related to the new coordinates by $\cos \Theta = J_2/J_1$ and $\Phi = 2\pi w_2$. The quantities v_1 and v_2 are angular frequencies defined by $v_1 = J_1/4\pi^3 a^2$ and $v_2 = 0$. The angular frequency v_2 equal to zero describes the degeneracy on a homogeneous sphere. These relations define the generating function S which performs a non-linear transformation. In the next sections, we shall add a subscript 0 to the function S to underline the zeroth-order approximation.

4 PERTURBATION SCHEME

In the previous section, we have introduced a canonical transformation which converts the great circle (the ray in a homogeneous Earth) into a single point: the pole of the great circle. This transformation has been known for a long time in plate tectonics.

Let us now consider a heterogeneous sphere where lateral variations are taken as perturbations from the homogeneous sphere. Constructing a canonical transformation which converts the ray trajectory into a single point is now too difficult. We simply want to construct a canonical transformation which converts the complex ray trajectory into a simpler trajectory (as a straight line in the following). In other words, we want to make corrections to the zeroth-order solution. We require only a transformation to simpler equations which might be approximately solved. Instead of using a generating function with mixed variables, known as the Von Ziepel's approach, we shall use the recent method of Lie series, expressing the generating function with respect to new variables. Nayfeh (1972) or Giacaglia (1972) give excellent reviews of the method and we refer the reader to them. The canonical transformation includes the previous transformation and an extra term. This term is neglected in the averaging principle when we go back to the original space, while the Lie series theory, which we describe in the following section, takes it into account in the way back.

5 HIGHER ORDER SOLUTIONS: LIE SERIES

Let us assume that the Hamiltonian can be expanded in the following form:

$$H = H_0 + \epsilon H_1 + \epsilon^2 H_2 + \dots \quad (24)$$

where ϵ is a small parameter. When ϵ is equal to zero, we have the homogeneous Hamiltonian H_0 with the previously defined generating transformation from $(\theta, \phi, p_\theta, p_\phi)$ to $(\beta_1^0, \beta_2^0, J_1^0, J_2^0)$, expressed in a subtle way with only new variables:

$$S_0[\tau, \theta(\tau, \beta_1^0, \beta_2^0, J_1^0, J_2^0), \phi(\tau, \beta_1^0, \beta_2^0, J_1^0, J_2^0), J_1^0, J_2^0]. \quad (25)$$

The variables θ and ϕ are given by relations (23). When ϵ is different from zero, the variables $(\beta_1^0, \beta_2^0, J_1^0, J_2^0)$ are no longer constant and depend on τ in a rather complicated way. A new transformation from $(\beta_1^0, \beta_2^0, J_1^0, J_2^0)$ to $(\beta_1, \beta_2, J_1, J_2)$ is introduced as a power series (Lie series) in ϵ .

$$S = S_0(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon S_1(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon^2 S_2(\tau, \beta_1, \beta_2, J_1, J_2) + \dots, \quad (26)$$

where S_1, S_2 are the generating functions in first and second order. The old constants are expanded with respect to the new

ones with a near identity transformation defined as infinitesimal transformations:

$$\begin{aligned}\beta_1^0 &= \beta_1 + \epsilon \beta_1^{01}(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon^2 \beta_1^{02}(\tau, \beta_1, \beta_2, J_1, J_2) + \dots, \\ J_1^0 &= J_1 + \epsilon J_1^{01}(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon^2 J_1^{02}(\tau, \beta_1, \beta_2, J_1, J_2) + \dots, \\ \beta_2^0 &= \beta_2 + \epsilon \beta_2^{01}(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon^2 \beta_2^{02}(\tau, \beta_1, \beta_2, J_1, J_2) + \dots, \\ J_2^0 &= J_2 + \epsilon J_2^{01}(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon^2 J_2^{02}(\tau, \beta_1, \beta_2, J_1, J_2) + \dots,\end{aligned}\tag{27}$$

with the following definitions:

$$\beta_i^{01} = \frac{\partial S_1}{\partial J_i}, \quad J_i^{01} = -\frac{\partial S_1}{\partial \beta_i}, \quad \beta_i^{02} = \frac{\partial S_2}{\partial J_i} + L_1\left(\frac{\partial S_1}{\partial J_i}\right), \quad J_i^{02} = -\frac{\partial S_2}{\partial \beta_i} - L_1\left(\frac{\partial S_1}{\partial \beta_i}\right).\tag{28}$$

The quantities (J_i, β_i) might be either (J_1, β_1) or (J_2, β_2) and L_1 is the Lie derivative defined by

$$L_n f = \frac{\partial f}{\partial \beta_i} \frac{\partial S_n}{\partial J_i} - \frac{\partial f}{\partial J_i} \frac{\partial S_n}{\partial \beta_i},\tag{29}$$

where summation over i is understood. The Lie derivative characterizes the speed at which f is modified when the coordinates are deformed by S_n . The transformed Hamiltonian K will be

$$K(\tau, \beta_1, \beta_2, J_1, J_2) = K_0(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon K_1(\tau, \beta_1, \beta_2, J_1, J_2) + \epsilon^2 K_2(\tau, \beta_1, \beta_2, J_1, J_2) + \dots.\tag{30}$$

The general theory of Lie series gives an equation for each order:

$$K_1 + \frac{\partial S_1}{\partial \tau} = H_1(\tau, \beta_1, \beta_2, J_1, J_2), \quad K_2 + \frac{\partial S_2}{\partial \tau} = H_2(\tau, \beta_1, \beta_2, J_1, J_2) + L_1(K_1 + H_1),\tag{31a}$$

$$(31b)$$

where terms H_i are expressed with new variables:

$$H_i[\tau, \theta(\tau, \beta_1, \beta_2, J_1, J_2), \phi(\tau, \beta_1, \beta_2, J_1, J_2), p_\theta(\tau, \beta_1, \beta_2, J_1, J_2), p_\phi(\tau, \beta_1, \beta_2, J_1, J_2)]\tag{32}$$

through relations (23) of old variables in terms of new ones. Higher order equations can be obtained from a recursion scheme which can be found in previously cited reviews. Because S is a canonical transformation, we still have the canonical equations

$$\begin{aligned}\dot{\beta}_1 &= \frac{\partial K}{\partial J_1} = \frac{\epsilon \partial K_1}{\partial J_1} + \epsilon^2 \frac{\partial K_2}{\partial J_1} + \dots, & \dot{J}_1 &= -\frac{\partial K}{\partial \beta_1} = -\frac{\epsilon \partial K_1}{\partial \beta_1} - \epsilon^2 \frac{\partial K_2}{\partial \beta_1} + \dots, \\ \dot{\beta}_2 &= \frac{\partial K}{\partial J_2} = \frac{\epsilon \partial K_1}{\partial J_2} + \epsilon^2 \frac{\partial K_2}{\partial J_2} + \dots, & \dot{J}_2 &= -\frac{\partial K}{\partial \beta_2} = -\frac{\epsilon \partial K_1}{\partial \beta_2} - \epsilon^2 \frac{\partial K_2}{\partial \beta_2} + \dots.\end{aligned}\tag{33}$$

These equations might be solved iteratively by assuming the following series expansion:

$$\beta_1 = \bar{\beta}_1 + \epsilon \beta_1^1 + \epsilon^2 \beta_1^2 + \dots, \quad J_1 = \bar{J}_1 + \epsilon J_1^1 + \epsilon^2 J_1^2 + \dots, \quad \beta_2 = \bar{\beta}_2 + \epsilon \beta_2^1 + \epsilon^2 \beta_2^2 + \dots, \quad J_2 = \bar{J}_2 + \epsilon J_2^1 + \epsilon^2 J_2^2 + \dots,\tag{34}$$

together with the initial conditions ($\tau = 0$),

$$\beta_1 = \bar{\beta}_1, \quad \beta_1^n = 0, \quad J_1 = \bar{J}_1, \quad J_1^n = 0, \quad \beta_2 = \bar{\beta}_2, \quad \beta_2^n = 0, \quad J_2 = \bar{J}_2, \quad J_2^n = 0, \quad n = 1, 2, \dots.\tag{35}$$

The quantities $\bar{\beta}_1, \bar{\beta}_2, \bar{J}_1, \bar{J}_2$ are the constant values of the zeroth-order solution (keep in mind that the coordinates $\beta_1^0, \beta_2^0, J_1^0, J_2^0$ are no longer constant for the heterogeneous sphere). Substituting these expansions into the canonical equations, we can solve the first-order equation by using the zeroth-order solution, the second-order equation by using the first-order solution and so on. This is the time-dependent perturbation procedure and the way we solve approximately the new canonical system. Of course, we have to choose the different terms of our generating function and, consequently, our new Hamiltonian. Because our zeroth-order solutions are periodic, we shall apply the procedure of cancelling secular terms in the generating function (see Nayfeh 1972). These secular terms will emerge in the transformed Hamiltonian. A more intuitive technique, called the averaging procedure, takes into account only the secular terms in the canonical equations and neglects the perturbation of the generating function: it has been applied to the same problem by Virieux (1989). Other choices of repartition between the Hamiltonian and the generating function are possible depending on the problem at hand.

To first order, integrating the Hamilton–Jacobi equation (31a) will give an analytical expression of S_1 . Computing derivatives of S_1 with respect to the new coordinates allows construction of $\beta_1^0, \beta_2^0, J_1^0, J_2^0$ from the relation (27). Inserting these expressions into the unperturbed transformation (23) will give the desired first-order perturbations of the solution. Computing the second-order solution is more involved because one has to evaluate Lie derivatives of H_1 and K_1 with respect to new coordinates but, in principle, the procedure is the same as for the first-order solution.

6 SPHERICAL HARMONICS EXPANSION

The Lie series approach is a very elegant method, but one has to construct analytically the functions introduced in the previous paragraph. If the square of the slowness is expressed in spherical harmonics, we can do this for a laterally heterogeneous sphere. The Hamiltonian H can be written as the sum of the homogeneous Hamiltonian H_0 and an extra term that we assume to be of first order and we shall expand it in the following form:

$$H_1(\theta, \phi, \cdot, \cdot) = \sum_{l,m} h_l^m Y_l^m(\theta, \phi), \quad (36)$$

where Y_l^m are fully normalized spherical harmonics (Backus 1964). The explicitly missing variables p_θ and p_ϕ are denoted by ' \cdot ' as commonly used in perturbation theory. Of course, we might take into account the amplitude of the different terms h_l^m and distribute them in different order terms. Because we have implemented numerically only the first-order perturbation, we do not discuss further such a strategy.

For numerical illustrations of this article, we choose an isotropic equivalent of the model of Montagner & Tanimoto (1990) expanded in spherical harmonics up to the azimuthal order 15 (Fig. 2). From the velocity expansion, we deduce the square of the slowness expansion related directly to the Hamiltonian expansion.

The term H_1 has to be expressed with the new variables, which is conveniently done with generalized spherical harmonics Q_l^{mn} (Backus 1964). One can find

$$H_1 = \sum_{l,m} h_l^m e^{im\Phi} \sum_n Q_l^{mn}(\Theta) e^{in\Psi} Q_l^{n0}\left(\frac{\pi}{2}, 2\pi w_1\right), \quad (37)$$

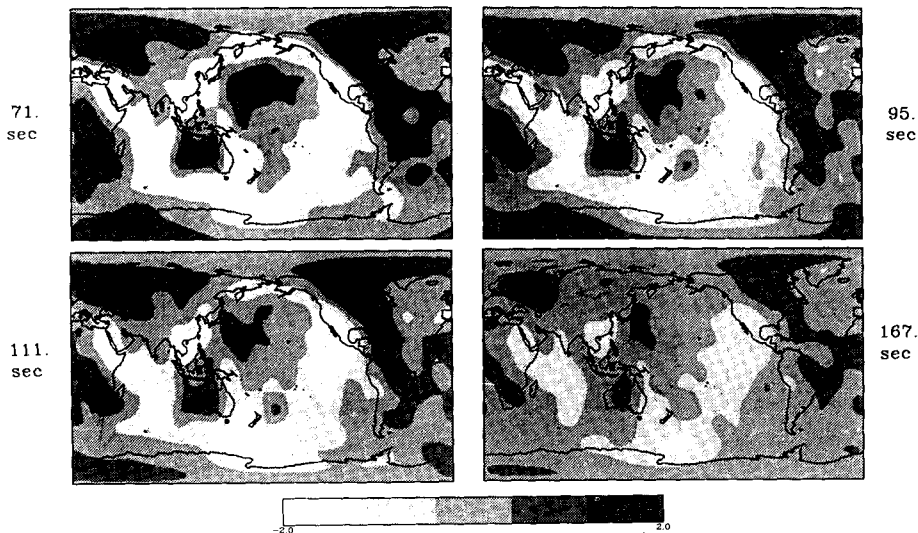
where the variable w_1 is equal to $v_1\tau + \beta_1$ and angles (Θ, Φ, Ψ) are the Euler angles from rotating the frame (θ, ϕ) to the (source, station) frame defined by the angles $(\pi/2, 2\pi w_1)$. The angles Θ, Φ contribute to the ray trajectory, while the angle Ψ is simply related to the origin of the parameter τ and can be set to zero without loss of generality. The relation (30a) gives

$$K_1 + \frac{\partial S_1}{\partial \tau} = \sum_{l,m} h_l^m e^{im\Phi} \sum_n Q_l^{mn}(\Theta) e^{in\Psi} Q_l^{n0}\left(\frac{\pi}{2}, 2\pi w_1\right). \quad (38)$$

Now, we select the slowly varying part, i.e. the secular terms, as the new Hamiltonian. These terms are defined by $n=0$ and the resulting Hamiltonian will be

$$K_1 = \sum_{l,m} h_l^m Q_l^{m0}(\Theta) e^{im\Phi} Y_l^0\left(\frac{\pi}{2}, 0\right), \quad (39)$$

PHASE VELOCITY of RAYLEIGH WAVES



Spherical harmonics decomposition

Angular order 15

Figure 2. Equivalent isotropic model of Montagner & Tanimoto (1990) in spherical harmonics expansion up to the 15th azimuthal order at different periods. The grey scale is the same for the different periods and will be used for the following figures.

which gives the following expression by transforming back to spherical harmonics:

$$K_1 = \sum_{l,m} h_l^m \frac{Y_l^0\left(\frac{\pi}{2}, 0\right)}{Y_l^0(0, 0)} Y_l^m(\Theta, \Phi), \quad (40)$$

already used by Virieux (1989). Integrating the Hamilton–Jacobi equation, one can deduce the first-order generating term S_1 :

$$S_1 = \sum_{l,m} h_l^m e^{im\Phi} \sum_{n,n \neq 0} Q_l^{mn}(\Theta) e^{in\Psi} \frac{Y_l^m\left(\frac{\pi}{2}, 2\pi w_1\right)}{i2\pi n v_1}, \quad (41)$$

which is the important contribution of the Lie series approach. A constant of integration $\mathcal{A}(\beta_1, \beta_2, J_1, J_2)$ must be introduced but one does not need to know it; only its derivatives with respect to coordinates have to be computed. The initial conditions provide us with these values. The first-order terms of the new canonical equations are obtained:

$$\dot{\beta}_1^1 = \frac{\partial K_1}{\partial J_1}, \quad \dot{J}_1^1 = -\frac{\partial K_1}{\partial \beta_1}, \quad \dot{\beta}_2^1 = \frac{\partial K_1}{\partial J_2}, \quad \dot{J}_2^1 = -\frac{\partial K_1}{\partial \beta_2}. \quad (42)$$

Because K_1 does not depend on β_1 , J_1^1 is constant which shows that J_1 is a first-order adiabatic invariant. This property stems from the action/angle property of the couple (w_1, J_1) (Virieux 1989). We integrate (42) with the zeroth-order solution on the RHS and obtain

$$\beta_1^1 = \delta v_1 \tau, \quad J_1^1 = 0, \quad \beta_2^1 = \delta v_2 \tau, \quad J_2^1 = \delta \mu_2 \tau, \quad (43)$$

where δv_1 , δv_2 and $\delta \mu_2$ are given by

$$\begin{aligned} \delta v_1 &= \sum_{l,m} h_l^m \frac{Y_l^0\left(\frac{\pi}{2}, 0\right)}{Y_l^0(0, 0)} \frac{\partial [Y_l^m(\Theta, \Phi)]}{\partial J_1} \Bigg|_{\Theta^0, \Phi^0}, & \delta v_2 &= \sum_{l,m} h_l^m \frac{Y_l^0\left(\frac{\pi}{2}, 0\right)}{Y_l^0(0, 0)} \frac{\partial [Y_l^m(\Theta, \Phi)]}{\partial J_2} \Bigg|_{\Theta^0, \Phi^0}, \\ \delta \mu_2 &= -\sum_{l,m} h_l^m \frac{Y_l^0\left(\frac{\pi}{2}, 0\right)}{Y_l^0(0, 0)} \frac{\partial [Y_l^m(\Theta, \Phi)]}{\partial \beta_2} \Bigg|_{\Theta^0, \Phi^0}. \end{aligned} \quad (44)$$

The quantities Θ^0 and Φ^0 are the pole coordinates for the zeroth-order solution. The total solution to this order is

$$\beta_1 = \bar{\beta}_1 + \beta_1^1 = \bar{\beta}_1 + \delta v_1 \tau, \quad J_1 = \bar{J}_1, \quad \beta_2 = \bar{\beta}_2 + \beta_2^1 = \bar{\beta}_2 + \delta v_2 \tau, \quad J_2 = \bar{J}_2 + J_2^1 = \bar{J}_2 + \delta \mu_2 \tau, \quad (45)$$

a result already obtained by Virieux (1989). Expressions (26) for β_1^0 , β_2^0 , J_1^0 and J_2^0 require partial derivatives of S_1 with respect to new coordinates, which are given in Appendix B. We finally go back to $(\theta, \phi, p_\theta, p_\phi)$ by inserting these values into the relation (23). This solution is different from the one constructed by the averaging principle (Virieux 1989) which neglects the contribution of the transformation S_1 . The solution, which was sensitive only to the even coefficients of the spherical harmonics expansion in the averaging procedure, is now modified by the odd coefficients through the generating function S_1 : a very attractive feature for inversion.

As a first example, we perform ray tracing from the ‘Gulf of Alaska’ earthquake of November 1987 to the GEOSCOPE station SSB with a take-off angle tangent to the great circle (coordinates of the GEOSCOPE stations used and the ‘Gulf of Alaska’ earthquake are shown in Table 1). We perform an entirely numerical ray tracing using a Runge–Kutta scheme of second order as well as the perturbed ray tracing. In Fig. 3, the coordinate frame is rotated in such a way that the source and the station lie on the equator. We consider the phase velocity model of Montagner & Tanimoto (1990) at 167 s on the left panel of Fig. 3, and this model amplified by an arbitrary factor of 1.5 on the right panel of Fig. 3. The relative variation of the heterogeneity velocity is 2 per cent in the true model and 3 per cent in the amplified model. The comparison between analytical and numerical ray tracing methods is surprisingly good taking into account that the analytical ray tracing in action/angle coordinates is simply a straight line (Fig. 3). This is the geometrical effect of the non-linear canonical transformations S_0 and S_1 .

As another example, we consider a R4 train for the same earthquake. We select the station GEOSCOPE INU and rotate continents in order to have source and station along the equator and we plot deviations up to 32° away from the great circle (Fig. 4). For the selected initial angle, the agreement between analytical and numerical rays is excellent for the first orbit. When the ray again traverses North America, a local perturbation with a strong gradient modifies the numerical ray, while the perturbed ray is insensitive to this gradient. The discrepancy increases at that time but overall features of rays are the same. As a rule of thumb, we might say that the product of velocity gradient and distance must be small for the perturbation technique to be valid.

Table 1. Coordinates of the GEOSCOPE stations used in this article, as well as the coordinates of the ‘Gulf of Alaska’ earthquake (1987).

Locations of Geoscope stations and earthquake used in this study	Latitude	Longitude
Station SSB	45.28	4.54
Station INU	35.35	137.04
Station CAY	4.95	-252.32
Gulf of Alaska earthquake (Nov. 1987)	58.17	-142.04

In two-point ray tracing, shooting at a given station adds another difficulty. The first step is an investigation of the branches arriving at the station. We proceed on a line perpendicular to the great circle defined by the couple (source, station) and, shooting systematically at different angles, we define the branches inside which the station is located. For the model of Montagner & Tanimoto (1990) at period of 167 s, branches are unusual, while, at shorter periods, they are more common. The previous example of GEOSCOPE station INU presents, for example, a caustic at about 15° off the great circle (Fig. 5). As we consider longer trains, the caustics at the source and at the antipole spread over a wider surface. Once branches are found, we simply solve the two-point ray tracing numerically by a modified regular falsi method for each branch and for the numerical and analytical methods of ray tracing independently. In doing it, we investigate other initial values of coordinates ($\beta_1, \beta_2, J_1, J_2$) for great circles nearby the one connecting the earthquake and the station.

Lie derivatives require derivatives with respect to Euler angles only, which can be analytically evaluated with a generalized spherical harmonics expansion. In other words, Lie derivatives can be expanded analytically on a generalized spherical harmonics basis. This feature of closure allows, in principle, the analytical construction of the solution up to second-order order from relations (28) and (31). By recurrence, the solution can be constructed to any order. Applying the theory to lateral heterogeneous models of the Earth will tell us whether or not the second-order solution is worth a numerical implementation.

Another alternative which might be numerically more efficient is updating the perturbation when one estimates that the deviations are too large. When variations $\delta v_1, \delta v_2$ or $\delta \mu_2$ induce deviations which are too large, we may compute the ray at only half the parameter τ of the station, for example. This point and its slowness vector define a great circle and one can

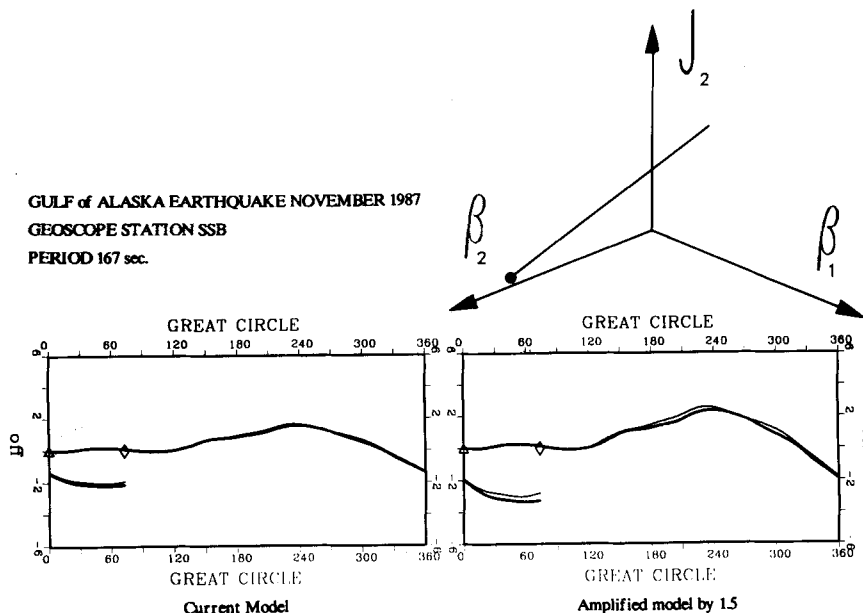


Figure 3. Comparison between analytical (thick line) and numerical (thin line) ray tracings for a given shooting angle at station SSB. We consider the model of Montagner & Tanimoto on the left panel. On the right panel, we amplify the perturbation of the model by a factor 1.5. The top panel presents the solution in the action/angle coordinates which is a simple straight line deduced from relation (44).

GULF of ALASKA EARTHQUAKE NOVEMBER 1987
 GEOSCOPE STATION INU : R4 train
 PERIOD 167 sec.

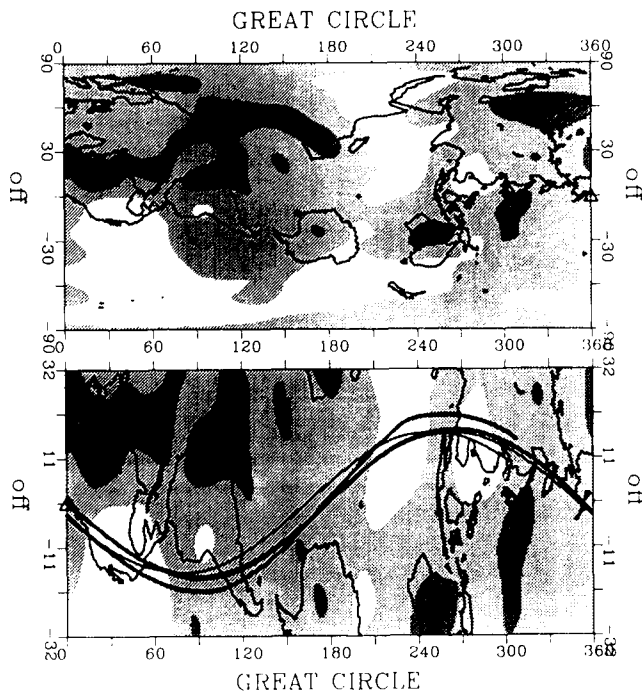


Figure 4. Selected shooting angle producing large deviations of the perturbed ray compared to the numerical ray tracing after one orbit. The INU station and the 'Gulf of Alaska' earthquake of 1987 are used for rotations.

GULF of ALASKA EARTHQUAKE NOVEMBER 1987
 GEOSCOPE STATION INU : R4 train
 PERIOD 167 sec.
 CAUSTICS PATTERN

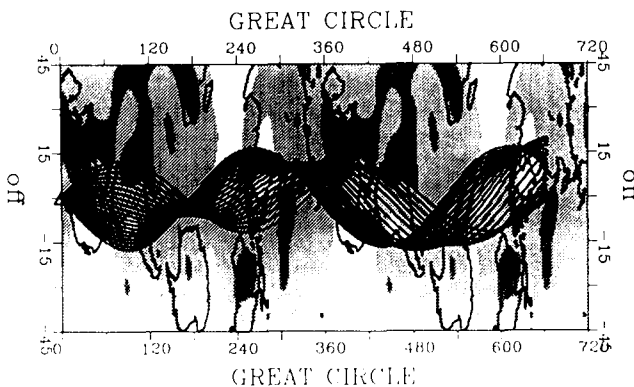


Figure 5. Presence of caustics for the model of Montagner & Tanimoto at period 167 s, near by the INU station. Please note the increasing surface associated with the source position as well as the antipole position.

perform the described perturbation starting from this new pseudo source, as we have done for the true source. This procedure will reduce our numerical efficiency but it will guarantee a given accuracy which can be controlled by the drift in the Hamiltonian: we are back to the updating taken at each step of any numerical ray tracing. However, the procedure will be a very efficient one, as suggested by Dahlen (1986).

7 PERTURBATION OF THE TRAVELTIME AND AMPLITUDE ESTIMATION

The Lie series approach enables us to estimate any quantities—traveltime, geometrical spreading, polarization, etc.—by expanding its perturbation with respect to the parameter ϵ . The extra work one has to accomplish is computing the Lie derivative of this quantity (Miller 1986). We shall concentrate on the two ingredients of synthesizing seismograms: traveltime and geometrical spreading.

The averaging procedure (Virieux 1989) does not provide a very efficient way to compute the traveltime, while the Lie series theory constructs an expression in powers of ϵ . Let us recall that the traveltime between point a and b on a sphere with a Hamiltonian H is given by the equation

$$T = \int_a^b p_\theta d\theta + p_\phi d\phi - H d\tau. \quad (46)$$

The term in $d\tau$ is often dropped because H is equal to zero for rays. We need it for the perturbation. Invoking the generating function S and the Hamilton–Jacobi equation gives

$$T = \int_a^b \frac{\partial S}{\partial \theta} d\theta + \frac{\partial S}{\partial \phi} d\phi + \frac{\partial S}{\partial \tau} d\tau = [S]_a^b. \quad (47)$$

Let us expand the traveltime for a heterogeneous sphere in powers of ϵ :

$$T = T_0 + \epsilon T_1 + \frac{1}{2}\epsilon^2 T_2 + \dots \quad (48)$$

The traveltime T_0 of the homogeneous sphere defined by the Hamiltonian H_0 will be $S_0(b) - S_0(a)$. The first variation of the traveltime can be written

$$\delta T = T - T_0 = [p_i \delta q_i]_a^b + \int_a^b \delta p_i \left(\frac{dq_i}{d\tau} - \frac{\partial H_0}{\partial p_i} \right) d\tau - \int_a^b \delta q_i \left(\frac{dp_i}{d\tau} + \frac{\partial H_0}{\partial q_i} \right) d\tau - \epsilon \int_a^b H_1 d\tau, \quad (49)$$

where implicit summation over i is understood and quantities (p_i, q_i) are either (p_θ, θ) or (p_ϕ, ϕ) . This expression is often expressed in terms of the Lagrangian (Nowack & Lyslo 1989). Because we have developed the Hamiltonian approach, we prefer to continue with it. Considering a ray for the Hamiltonian H_0 connecting points a and b , the traveltime reduces to the last term. We deduce the contribution T_1 of the traveltime Lie series:

$$T_1 = - \int_a^b H_1 d\tau = - \int_a^b \left(\frac{\partial S_1}{\partial \tau} + K_1 \right) d\tau. \quad (50)$$

Noting that K_1 is τ -independent, we integrate and end up with the simple expression

$$T_1 = -[S_1]_a^b - K_1[\tau(b) - \tau(a)]. \quad (51)$$

From the traveltime, one deduces the apparent phase velocity by dividing the traveltime with the distance between the source and the station. For arbitrary (source/station) couples, we compute the relative error of the apparent velocity obtained by the perturbed ray tracing and the numerical procedure in Fig. 6. We found a percentage error lower than 0.2 per cent for R1 trains and less than 0.6 per cent for R4 trains.

The lateral heterogeneities introduce a focusing/defocusing effect which modifies the geometrical spreading. Although one might compute the geometrical spreading by perturbation using Lie series, we estimate this effect numerically during our shooting procedure. We slightly perturb the shooting angle δi and compute the position shift $\delta \theta$ at the station. We deduce an amplification compared to the homogeneous sphere defined by

$$A = \frac{\sin \Delta}{\delta \theta / \delta i}, \quad (52)$$

where Δ is the angular distance between the source and the station. This approach is the quickest way to estimate quantities in order to synthesize seismograms. The other alternative is computing the Jacobian between the two coordinate systems we are using. The Jacobian requires many more trigonometric functions than the ones needed for a ray. For amplitude inversion, we would have to estimate this Jacobian related to the more involved analytical Lie series in order to compute partial derivatives.

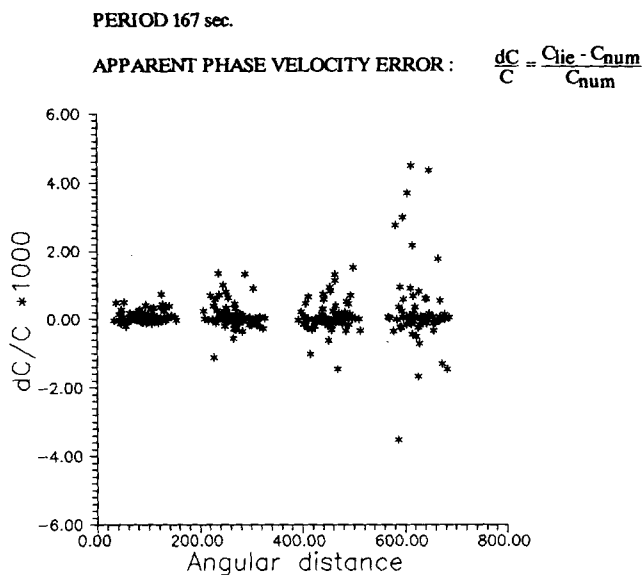


Figure 6. Comparison of traveltimes or apparent velocities for many couples (source, station) obtained by the perturbed ray tracing and analytical ray tracing. We define the apparent phase velocity by C_{lie} for the perturbed ray tracing and by C_{num} for the numerical ray tracing.

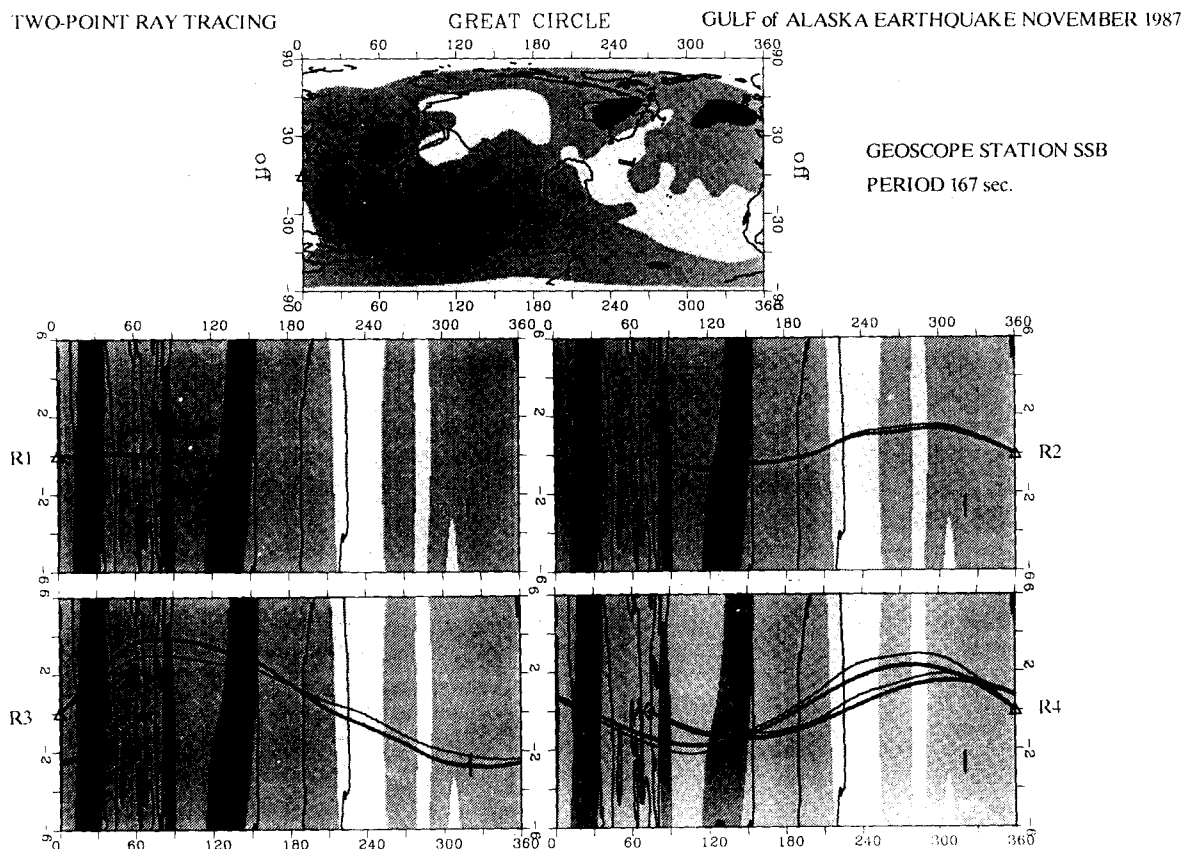


Figure 7. Comparison of analytical (thick line) and numerical (thin line) ray tracings at station SSB for the 'Gulf of Alaska' earthquake (1987). Small deviations compared to the great circle are obtained.

8 AN EXAMPLE: THE 'GULF OF ALASKA' EARTHQUAKE OF NOVEMBER 1987

We have selected the 'Gulf of Alaska' earthquake of November 1987 which presents strong amplitude anomalies in its long-period seismograms. These anomalies might in part reflect the off great circle path propagation of wavetrains. We perform ray tracing to different GEOSCOPE stations and find good agreement between numerical ray tracing and perturbed ray tracing at a period of 167 s (see previous section).

Figure 7 shows rays arriving at the station SSB, where deviations are small, while the rays arriving at the station INU show large deviations with respect to the great circle (Fig. 8). We still obtain good agreement except for the R4 train where we underestimate the shooting angle. For this last ray, the reinitialization would guarantee a given accuracy compared to the numerical ray tracing.

A very interesting result is obtained at the station CAY. For the PREM model, we compute the vertical seismogram using normal modes with isolated multiplets. We compute also the seismogram for the asymptotic normal modes summation of Romanowicz (1987) where we consider lateral variations of the model used in this article. One can see the defocusing of R3 and R5, as well as the focusing of R4 and R6 predicted by the asymptotic theory (Fig. 9). These variations are supported by the true seismogram. The anomalous small R1 train is probably due to the nodal character of this path. The focusing/defocusing effect is predicted by ray tracing when we choose rays starting tangent to the great circle (Table 2). When shooting is performed for the different trains, we found that the expected amplification of R4 is replaced by a strong deamplification. This is not a bias coming from our perturbed ray tracing, because the numerical ray tracing finds the same result. This prediction of ray tracing might imply a need for better estimations of perturbation anomalies, as noted also by Lay & Kanamori (1985), Schwartz & Lay (1985) and Woodhouse & Wong (1986).

9 CONCLUSIONS

We have presented the Lie series method for tracing rays on a heterogeneous sphere. The approximate solution is expressed analytically when the global representation in spherical harmonics of the heterogeneity is used. The ray, usually sensitive to the even part of the expansion, is now deformed also by the odd part which makes this theory very attractive for inversion. The perturbations of the traveltimes are analytically computed. Focusing and defocusing effects are, at the present stage, estimated

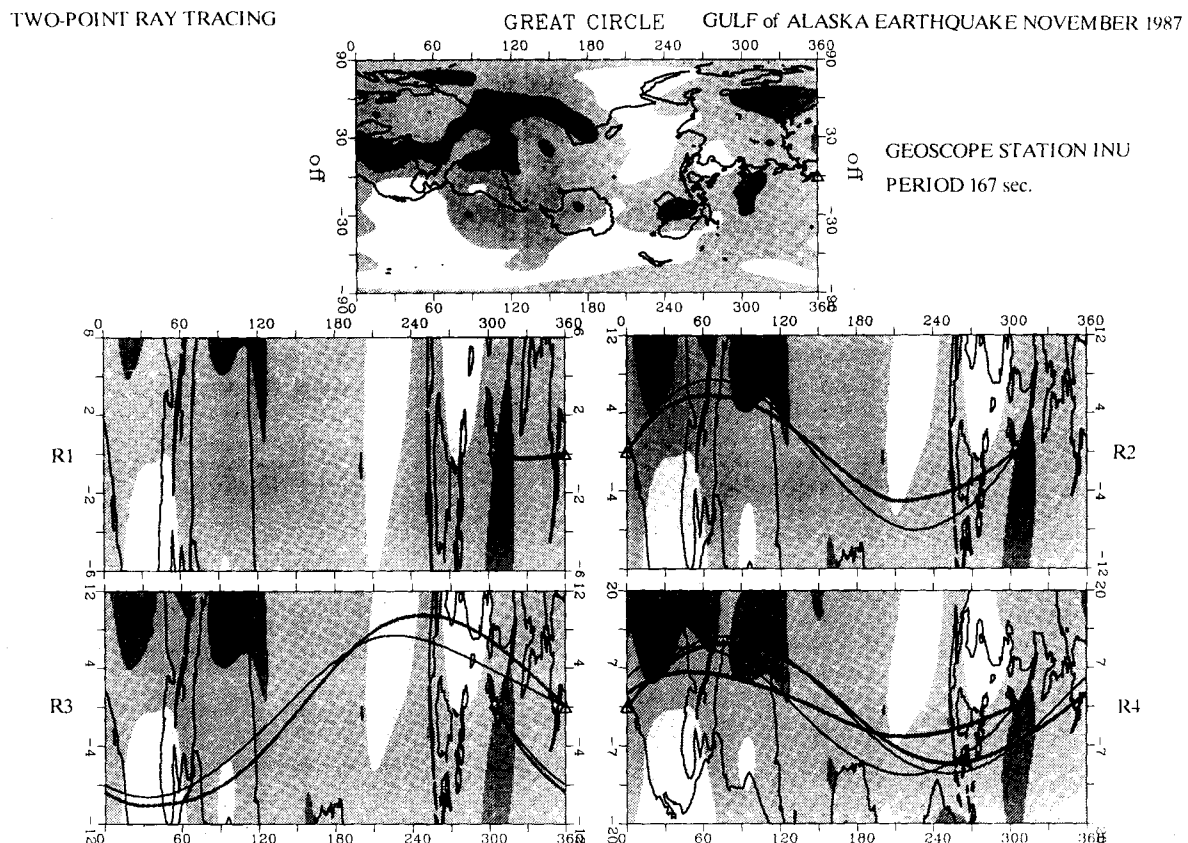


Figure 8. Comparison of analytical (thick line) and numerical (thin line) ray tracings at station INU for the 'Gulf of Alaska' earthquake (1987). Large deviations compared to the great circle are obtained. Please note the different scales used in the panels.

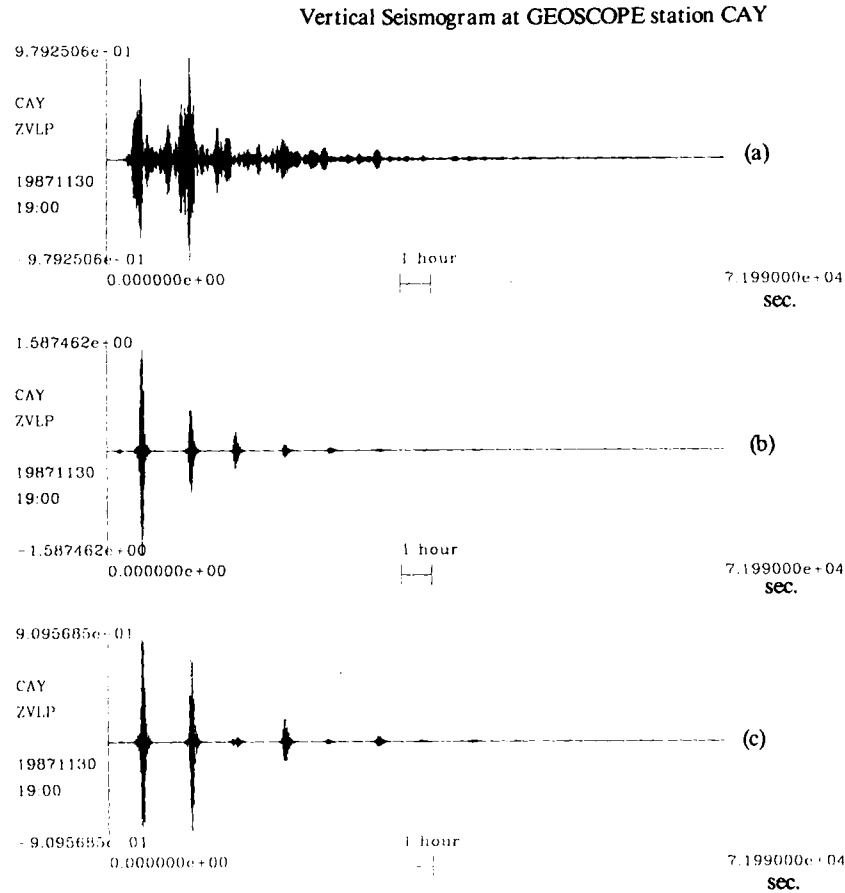


Figure 9. Vertical seismograms at station CAY for the Alaska earthquake (1987): (a) data filtered around 167 s, (b) isolated multiplet summation with the same filtering as the data and (c) asymptotic theory of normal modes with the same filtering as the data. Note the focusing and defocusing effect on the different trains.

numerically. Because the solution is computed only at the station position, the ray tracing is an order of magnitude faster than usual numerical ray tracing.

This ray tracing performs correctly for periods greater than 150 s. For shorter periods where gradients of perturbations are higher, the solution is still better than the great circle but shows significant discrepancies in terms of shooting angles and amplitudes. The computational reinitialization of the ray is a procedure that will solve this problem, but that will reduce the efficiency. In any case, it will be faster than any numerical scheme and will allow partial derivatives to be computed.

For the specific example of the ‘Gulf of Alaska’ November 1987 earthquake, we have found that the deviations of rays from the great circle can be significant. The perturbed ray tracing predicts accurately the traveltimes as well as a good

Table 2. Comparison between quantities obtained by the perturbed ray tracing and by the numerical ray tracing at station CAY. Amplifications for shooting angles tangent to the great circle are also given.

Numerical ray tracing			Perturbed ray tracing			Amplification for a shooting angle tangent to the great circle			
	Travel-time	Amplification	Shooting angle	Travel-time	Amplification	Shooting angle			
R1	2150 sec.	0.78	3.25°	R1	2151 sec.	0.85	3.16°	R1	0.74
R2	6913 sec.	1.01	-1.04°	R2	6910 sec.	1.12	-1.06°	R2	1.09
R3	11213 sec.	0.56	5.48°	R3	11214 sec.	0.59	5.98°	R3	0.51
R4	15978 sec.	0.55	-4.18°	R4	15962 sec.	0.62	-7.43°	R4	1.32

approximation of the shooting angle and the amplification at different stations compared to numerical ray tracing at period of 167 s. The observed defocusing/focusing effect is not often predicted by current phase velocity models (especially when we perform the two-point ray tracing). This trend argues for a better resolution of global models.

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APPENDIX A: GENERATING FUNCTION S

We describe the standard systematic procedure for constructing the generating function S when the Hamiltonian fulfils the separability conditions. Let us recall the structure of the Hamiltonian for a homogeneous sphere:

$$H(\theta, -, p_\theta, p_\phi) = \frac{1}{2} \left(\frac{p_\theta^2}{a^2} + \frac{p_\phi^2}{a^2 \sin^2 \theta} - u_0^2 \right) = E. \quad (\text{A1})$$

We assume the additive separability for the function S :

$$S(\tau, \theta, \phi, J_1, J_2) = W(\theta) + V(\phi) - E\tau. \quad (\text{A2})$$

The implicit parameter ϕ will give a very simple function $V(\phi)$ equal to $J_2/2\pi\phi$. We introduce the expression of S in the Hamilton–Jacobi equation and get the following expression:

$$H\left(\theta, -, \frac{dW}{d\theta}, \frac{J_2}{2\pi}\right) = E, \quad (\text{A3})$$

from which one obtains the function W by quadrature:

$$W(\theta) = \pm \int d\theta \sqrt{2E + u_0^2 - \frac{J_2^2}{4\pi^2 a^2 \sin^2 \theta}}. \quad (\text{A3})$$

In a natural way, we define $J_1^2/4\pi^2 a^2$ as $2E + u_0^2$ and present the final expression of S :

$$S(\tau, \beta_1, \beta_2, J_1, J_2) = \pm \frac{1}{2\pi a} \int d\theta \sqrt{J_1^2 - \frac{J_2^2}{\sin^2 \theta}} + \frac{J_2}{2\pi} \phi - \frac{J_1^2}{8\pi^2 a^2} \tau - \frac{1}{2} u_0^2 \tau. \quad (\text{A4})$$

The conjugate variables of J_1 and J_2 are given by

$$\beta_1 = \frac{\partial S}{\partial J_1} = \pm \frac{J_1}{2\pi a} \int \frac{d\theta}{\sqrt{J_1^2 - \frac{J_2^2}{\sin^2 \theta}}} - v_1 \tau, \quad \beta_2 = \frac{\partial S}{\partial J_2} = \mp \frac{J_2}{2\pi a} \int \frac{d\theta}{\sin^2 \theta \sqrt{J_1^2 - \frac{J_2^2}{\sin^2 \theta}}} + \frac{\phi}{2\pi}, \quad (\text{A5})$$

with v_1 given in the text. Quadratures are easy to solve (Goldstein 1980, p. 481) and this gives θ and ϕ with respect to coordinates $(\beta_1, \beta_2, J_1, J_2)$, while p_θ and p_ϕ come directly from the definition of J_1 and J_2 . We obtain the transformation defined by equations (23).

APPENDIX B: PARTIAL DERIVATIVES OF THE FUNCTION S_1

We use implicit summation over m and n between $-l$ and $+l$ and introduce the natural variable $z = \cos \Theta$ involved in generalized spherical harmonics Q_l^{mn} . The four partial derivatives are given by

$$\frac{\partial S_1}{\partial \beta_1} = \sum_{l,m} h_l^m e^{im\Phi} \sum_{n,n \neq 0} Q_l^{mn}(z) e^{in\Psi} \frac{Y_l^n\left(\frac{\pi}{2}, w_1\right)}{v_1}, \quad \frac{\partial S_1}{\partial \beta_2} = 2\pi \sum_{l,m} m h_l^m e^{im\Phi} \sum_{n,n \neq 0} Q_l^{mn}(z) e^{in\Psi} \frac{Y_l^n\left(\frac{\pi}{2}, w_1\right)}{2\pi n v_1}, \quad (\text{B1})$$

$$\frac{\partial S_1}{\partial J_1} = \frac{\partial S_1}{\partial z} \frac{\partial z}{\partial J_1} + \frac{\partial S_1}{\partial v_1} \frac{\partial v_1}{\partial J_1}, \quad \frac{\partial S_1}{\partial J_2} = \frac{\partial S_1}{\partial z} \frac{\partial z}{\partial J_2},$$

with the following partial derivatives:

$$\frac{\partial z}{\partial J_1} = -\frac{J_2}{J_1^2}, \quad \frac{\partial z}{\partial J_2} = \frac{1}{J_1}, \quad \frac{\partial v_1}{\partial J_1} = \frac{v_1}{J_1}, \quad (\text{B2})$$

and

$$\frac{\partial S_1}{\partial z} = \sum_{l,m} h_l^m e^{im\Phi} \sum_{n,n \neq 0} W(z) e^{in\Psi} \frac{Y_l^n\left(\frac{\pi}{2}, 2\pi w_1\right)}{i2\pi\nu_1}, \quad (\text{B3})$$

$$\frac{\partial S_1}{\partial \nu_1} = \frac{\tau}{\nu_1} \sum_{l,m} m h_l^m e^{im\Phi} \sum_{n,n \neq 0} Q_l^{mn}(z) e^{in\Psi} \frac{Y_l^n\left(\frac{\pi}{2}, w_1\right)}{2\pi n \nu_1} - \frac{S_1}{\nu_1}. \quad (\text{B4})$$

The expression $\partial S_1/\partial \nu_1$ has a term linear in τ which gives a surprising added secular contribution to β_1^0 . This contribution was ignored in the averaging procedure. The function $W(z)$ is the combination $[q^+ Q_l^{m(n-1)}(z) + q^- Q_l^{m(n+1)}(z)]$ where factors q^+ and q^- are given respectively by $\sqrt{(1-n)(1+n+1)}$ and $\sqrt{(1+n)(1-n+1)}$ (Vilenkin 1969, p. 136).

The values of derivatives of S_1 at the origin of the ray have to be subtracted at any other position on the ray. This cancels the effect of the constant of integration \mathcal{A} .