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Calculation of 2D ray-fields in smooth media using a pseudo-spectral expansion technique

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ABSTRACT

A new method for calculating ray-fields in smooth media is presented. The method is based on the observation that in these media ray variables such as position, slowness and travel time are smooth functions of the ray parameters. The dependence of the rays on the initial conditions is approximated using a pseudo-spectral expansion in terms of Chebyshev polynomials. The smoothness of the functions guarantees exponential convergence of the expansion and thus a relatively low number of evaluations of the ray equations. The result of a calculation is a continuous analytic representation of the ray-field which may subsequently be used to project ray information onto a grid defined in the medium, to generate tables of possibly multi-valued travel times and amplitudes for use in imaging and source location algorithms. In order to overcome difficulties of the method related to variations in geometrical spreading over the range of initial conditions a new ray-field parameterization was conceived. This parameterization allows a more efficient calculation of the ray field and its projections by abandoning the ray itself as the basis of the expansion.

Key words: ray tracing, migration, pseudo-spectral expansions

1 INTRODUCTION

A central part of the migration or inversion algorithms for seismic reflection data is the calculation of Green's functions for the wave equation. The Green's functions are required for every combination of a surface position, either source or receiver, and a grid point in the subsurface. To adequately image the subsurface, the subsurface grid has to be fairly dense, and especially in 3D applications the calculations is expensive. Moreover, the velocity structures of the media of interest are usually complex enough for the wave field to develop caustics and associated multi-pathing. It has been established that for accurate imaging it is essential to take more than just the first arrival into account (Geoltrain & Brac, 1993).

Ray theory provides the most efficient methods for the calculation of the multi-valued Green's functions on a grid. Within the ray-based methods various approaches are possible. Classical two point ray tracing is slow and the search for multiple arrivals boils down, in

practice, to an exhaustive search. More modern methods instead use a two-stage process consisting of first shooting with a range of initial conditions, and then projecting onto the grid. Paraxial ray methods use perturbations to project ray information on the grid positions. Due to the ambiguity of the projection, which is basically an extrapolation, this method is not suitable for dealing with multi-pathing. It also has problems finding arrivals in regions of large geometrical spreading. The wavefront construction techniques (Vinje *et al.*, 1993; Lambaré *et al.*, 1996) do not have these problems and are currently the most efficient methods for this purpose.

In this paper we propose a new method for the calculation of ray fields, based on a pseudo-spectral expansion technique. Similar to the wavefront construction techniques this method takes the continuity of the ray-field into account. This is the property that allows it to calculate all arrivals onto a grid without redundancy or ambiguity. The main difference with the wavefront con-

struction techniques is that it uses global rather than local approximations of the wavefront. This is justified by the smoothness of the ray-field in terms of the ray parameters. The uniform exponential convergence of the pseudo-spectral expansion allows the ray-field to be approximated using much less evaluation points. The result of a calculation is an analytic expression for the ray-field which allows various posterior calculations on the ray-field such as projection on a grid, location of caustics and intersection with interfaces.

2 KINEMATIC RAY TRACING IN THE HAMILTONIAN FORMULATION

The ray equations may be derived from various physical principles associated with wave propagation (Červený, 2001). Fermat's principle leads directly to the Lagrangian and Hamiltonian formulations of ray theory through an analogy with Hamilton's principle of classical mechanics (Lanczos, 1986; Goldstein, 1980). The reconciliation with wave theory is achieved by a high frequency asymptotic analysis on the acoustic or elastic wave equation. This leads to the eikonal equation, a nonlinear ordinary differential equation for the phase of a wave. The rays may be found from this equation using the method of characteristics (Bleistein, 1984). This method again leads to the Hamiltonian formulation of ray tracing by identifying the Hamiltonian with a form of the eikonal equation.

As the point of departure we choose the eikonal equation:

$$\nabla T \cdot \nabla T = u^2, \quad (1)$$

where T is the phase or travel time of a wave, and $u = u(\mathbf{r})$ is the slowness of the medium, or inverse velocity. For the solution of this equation using the method of characteristics the reader is referred to (Bleistein, 1984). Following (Červený, 2001) we recognize that any solution which satisfies the eikonal equation (1) also satisfies the more general equation

$$F(\mathbf{p} \cdot \mathbf{p}) = F(u^2), \quad (2)$$

in which we define the slowness vector $\mathbf{p} = \nabla T$ and $F(x)$ is a continuous function with continuous first and second derivatives for which the first derivative $F'(x)$ satisfies $x F'(x) > 0$ in the region of interest. Although this equation has exactly the same solutions as (1), the characteristics and thus the rays calculated from it will in general have different parameterizations. It is this property which we can use for the definition of different Hamiltonians which yield the same ray solutions, but with different parameterizations.

A wide range of Hamiltonians is given by (Červený, 2001):

$$\mathcal{H}_n(\mathbf{r}, \mathbf{p}) = \frac{1}{n} \left\{ (\mathbf{p} \cdot \mathbf{p})^{n/2} - u^n(\mathbf{r}) \right\}, \quad (3)$$

with \mathbf{r} the ray position and n an integer value. This expression is also valid for the limit $n \rightarrow 0$. In that case the l'Hôpital rule gives

$$\mathcal{H}_0(\mathbf{r}, \mathbf{p}) = \frac{1}{2} \ln \left(\frac{\mathbf{p} \cdot \mathbf{p}}{u^2(\mathbf{r})} \right). \quad (4)$$

In the Hamiltonian formulation rays are found as a function of some independent parameter σ by integrating the canonical equations

$$\frac{d\mathbf{r}}{d\sigma} = \nabla_{\mathbf{p}} \mathcal{H}, \quad \frac{d\mathbf{p}}{d\sigma} = -\nabla_{\mathbf{r}} \mathcal{H}, \quad \frac{dT}{d\sigma} = \mathbf{p} \cdot \frac{d\mathbf{r}}{d\sigma} \quad (5)$$

combined with proper initial conditions, where we denote differentiation to space coordinates by $\nabla_{\mathbf{r}}$, and differentiation with respect to slowness \mathbf{p} by $\nabla_{\mathbf{p}}$. The symbol T denotes the travel time along the ray. Together, \mathbf{r} and \mathbf{p} span a $2N$ dimensional space (with N the dimension of the medium) which is referred to as *phase space*. From equations (5) it is clear that the dimension and thus the physical meaning of the independent parameter follows from the dimension of \mathcal{H} . The choice $n = 0$ from equation (4) gives a dimensionless Hamiltonian which corresponds to time t as the independent parameter. Similarly, $n = 1$ yields a parameter that corresponds to the arc length s along the ray, and both $n = 2$ and $n = -1$ provide other independent parameters which have been used in the past. For arbitrary values of n , even for $n = 0$, the ray equations read:

$$\frac{d\mathbf{r}}{d\sigma_n} = u^{n-2} \mathbf{p}, \quad \frac{d\mathbf{p}}{d\sigma_n} = u^{n-1} \nabla_{\mathbf{r}} u, \quad \frac{dT}{d\sigma_n} = u^n. \quad (6)$$

The subscript n at σ_n denotes the dependence of the physical meaning of σ on n . As argued before, $\sigma_0 \equiv t$, and $\sigma_1 \equiv s$. In the derivation of (6) we have substituted the eikonal equation $\mathbf{p} \cdot \mathbf{p} = u^2$ wherever applicable.

Various other choices of the Hamiltonian are possible, some of which reduce to the same ray equations. Appendix A provides a Hamiltonian formulation which is different from the ones above in that it uses one of the space coordinates as parameter along the ray.

3 RAY-FIELDS

The term ray-field is used to denote an ensemble of rays corresponding to a continuous set of initial conditions, such as all rays emanating from a single point source, or all rays extending from an initial surface. These initial conditions may be defined in terms a set of parameters, the number of which is one less than the dimension of the medium. For a point source in a two dimensional medium a natural choice for this single parameter would be the take-off angle. Together with the independent parameter along the ray these initial condition parameters are called the *ray parameters*. The number of ray parameters for a ray-field is equal to the dimension of the medium. For convenience the parameter along the ray will henceforth be called *flow parameter*, while the

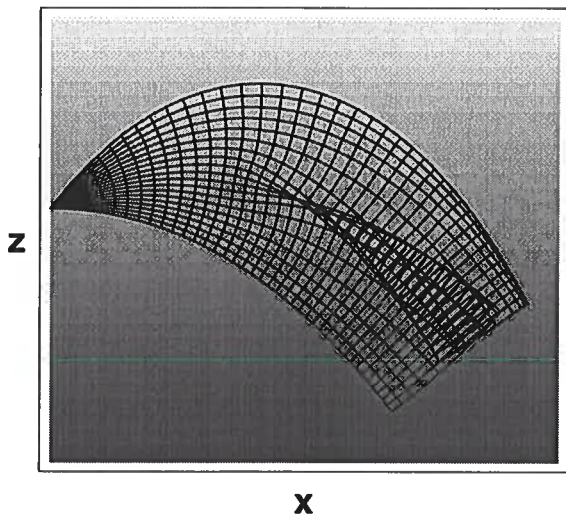


Figure 1. A ray ensemble from a point source in a simple velocity structure. The velocity structure consists of a constant gradient of the slowness pointing in negative z -direction, and on top of that a slow anomaly. This anomaly leads to folding of the ray-field and consequently triplication of the number of arrivals in the region enclosed by the cuspid caustic.

term *ensemble parameters* will stand for the rest of the set.

If the medium is smooth each ray variable (position, slowness, travel time, etc.) is a smooth function of the flow parameter. Similarly, if the initial conditions are smooth functions of the ensemble parameters, the entire ray-field can be described by smooth functions of the ray parameters. In spatially varying velocity structures, rays within the ray-field eventually cross in physical space and the number of rays crossing a particular point of space may change from place to place (see Figure 1). The information we are interested in is usually a map of certain ray information on physical space. If rays cross in physical space, these maps will be multi-valued and discontinuous. It is important to realize that these irregularities are caused by the projection of the ray information onto physical space, not by discontinuities in the ray field. The ray-field defines a smooth, N -dimensional manifold in $2N$ -dimensional phase space (see Figure 2). In terms of differential geometry this manifold has the properties of a Lagrangian submanifold, which is why it is often called the Lagrangian manifold of the ray tracing system. The projection of this manifold onto physical space yields the rays and the ray field maps. The singularities of the mapping, i.e. the edges of the folds, correspond to the caustics of the ray-field. For more details on the geometry of ray-fields in phase space the reader is referred to (Kendall & Thomson, 1993) or (Hanyga, 1984) in the geophysical literature, or (Guillemin & Sternberg, 1977) for a thorough mathematical treatment.

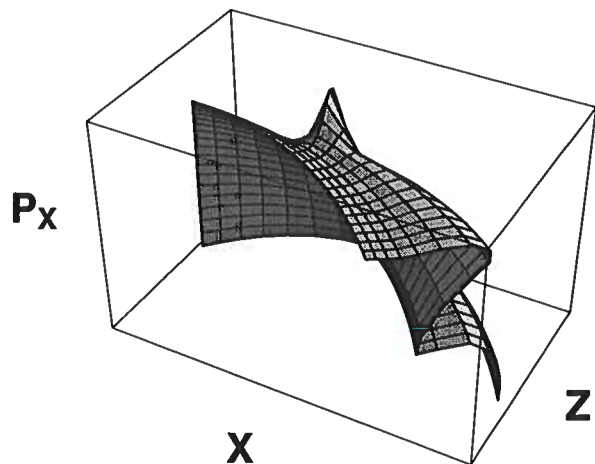


Figure 2. The same ray-field as in Figure 1, but now in a 3D projection of the 4D phase space consisting of the physical space at the horizontal plane and the x -component of the slowness along the vertical axis. The rays span a smooth manifold in this subspace, the projection of which onto physical space gives the rays of Figure 1.

4 RAY-FIELD EXPANSION

In this section we write the phase space ray position, which contains both spatial coordinates and slowness components, as a single vector \mathbf{v} :

$$\mathbf{v} = \begin{pmatrix} \mathbf{r} \\ \mathbf{p} \end{pmatrix}. \quad (7)$$

The system of ray equations 5 is summarized by

$$\frac{d\mathbf{v}}{d\sigma} = \mathbf{F}(\mathbf{v}), \quad (8)$$

with \mathbf{F} an unspecified right hand side vector which depends on the choice of Hamiltonian (see Section 2).

In the following we consider the ray-field emitted by a point source in a 2D medium, so we need only one parameter (ξ) to parameterize the initial conditions. The usual approach is to solve (8) for a discrete set of values of ξ . To get a continuous estimate of the ray-field we expand the ξ -dependence into a set of basis-functions $B_j(\xi)$, which we assume to be orthonormal with respect to an associated inner product:

$$\int_{\xi_0}^{\xi_1} B_i(\xi) B_j(\xi) W(\xi) d\xi = \delta_{ij}, \quad (9)$$

where $W(\xi)$ is a weighting function, and δ is the Kronecker delta. The ray-field may thus be expressed as a series expansion:

$$\mathbf{v}(\sigma, \xi) = \sum_{j=0}^N \mathbf{c}_j(\sigma) B_j(\xi). \quad (10)$$

The vector of coefficients \mathbf{c} , which depends on σ , may be calculated using the relation

$$\mathbf{c}_j(\sigma) = \int_{\xi_0}^{\xi_1} \mathbf{v}(\sigma, \xi) B_j(\xi) W(\xi) d\xi. \quad (11)$$

In order to trace the coefficients \mathbf{c}_j , the right hand side of equation (8) has to be expanded likewise, with coefficients $\mathbf{f}_j(\sigma)$. This gives a differential equation for the coefficients:

$$\frac{d\mathbf{c}_j(\sigma)}{d\sigma} = \mathbf{f}_j(\sigma). \quad (12)$$

If the parameter σ along the ray corresponds to time, then for a constant σ , $\mathbf{r}(\sigma, \xi)$ describes the position of a wavefront. In the following we call a curve of constant σ a “ σ -front.” Tracing an expanding σ -front with a certain accuracy requires in general a progressing number of coefficients. The actual number of coefficients depends on the complexity of the σ -front, which is directly related to the complexity of the traversed medium.

5 THE PSEUDO-SPECTRAL METHOD

Global expansion methods have become popular for the solution of partial differential equations, in which field they are collectively known as spectral methods. The usual approach is to expand the spatial dependence of the desired solution in a set of suitable basis functions, ending up with a set of ordinary differential equations for the temporal dependence. Our application is slightly different, for we expand the dependence on the initial conditions for an ordinary differential equation. Nevertheless, many aspects of both problems are the same, and we may take advantage of the existing literature (Boyd, 2000; Fornberg, 1996). This section provides a short summary of the basic principles of spectral methods.

Given an equation

$$Lu = f(x), \quad (13)$$

where L is an operator, which is not necessarily linear, the solution is approximated by a series expansion

$$u(x) \approx u_N(x) = \sum_{n=0}^N a_n \phi_n(x). \quad (14)$$

Substitution of the series in the solution generates a residual function R :

$$R(x; a_n) = Lu_N - f. \quad (15)$$

Spectral methods are designed to find a series of coefficients a_n in such a way that the residual function is made as small as possible. The different spectral and pseudo-spectral techniques differ mainly in their way of minimizing R .

The basic ingredients of a spectral method are:

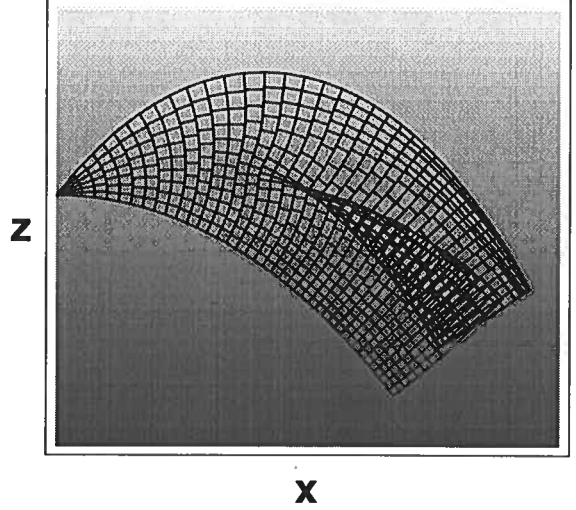


Figure 3. The same ray-field as in Figure 1, but now traced using the ray-field expansion technique.

- A suitable set of basis functions. The most important properties are completeness, rapid evaluation, rapid derivation, rapid convergence.
- An error criterion (norm), needed to quantify the quality of the approximation.
- An algorithm to determine the coefficients.

The most common basis functions used are Chebyshev polynomials, the default choice for functions on finite intervals, and trigonometric functions (Fourier) for periodic functions. Different sets are useful in case of special geometries (e.g. spherical harmonics) or unbounded intervals (e.g. Laguerre functions).

Since the quality of the approximation is usually determined by the maximum error or the entire interval, the norm of choice would be the L_∞ - or sup-norm. The problem with this norm is that is difficult to deal with analytically. The most practical norm is the L_2 - or least-squares-norm, because it allows fast algorithms for the determination of coefficients, especially if the basis set is orthogonal. Fortunately there are ways to relate least squares error estimates to sup-norm estimates.

Basically there are two types of algorithms to determine the expansion coefficients. The classical methods (Galerkin, Lanczos tau) minimize the residual function by making it orthogonal to as many basis functions as possible. The modern collocation methods minimize the residual by making it zero at a finite set of points. The latter methods are usually referred to as pseudo-spectral methods. Choosing the right set of collocation points makes the pseudo-spectral methods equivalent to the classical methods.

For our application we choose to use the pseudo-spectral technique in combination with Chebyshev polynomials. This provides uniform exponential convergence

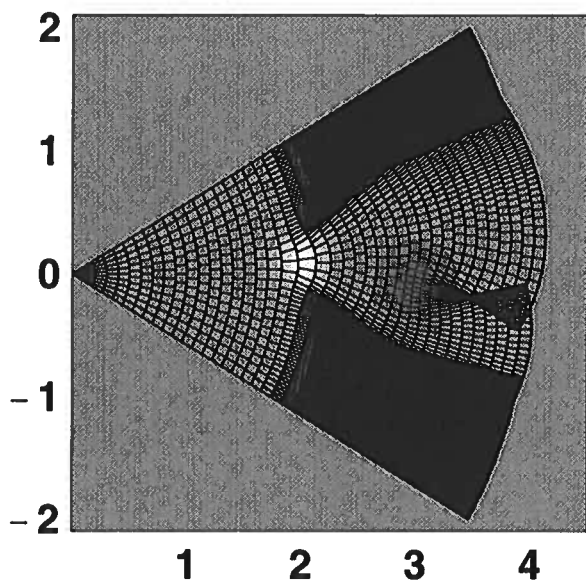


Figure 4. An example of how large variations in geometrical spreading lead to a non-uniform sampling in the ray-field expansion approach.

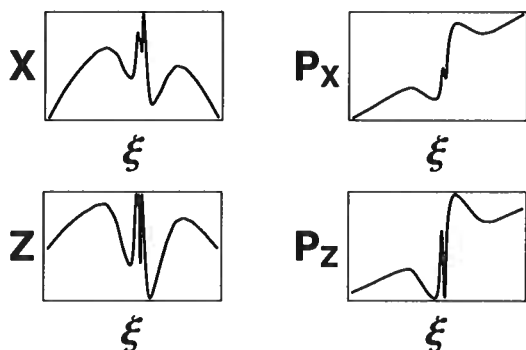


Figure 5. Graphs of the ray-field variables as a function of ensemble parameter ξ . The graphs correspond to the last wavefront plotted in Figure 4

in the sup-norm. Algorithms for the Chebyshev expansion may be found in (Press *et al.*, 1992).

6 EXAMPLES

Figure 3 shows the application of our wave field expansion technique to the same model studied in Figures 1 and 2. Time was used as flow parameter and the integration of the coefficients in time was performed using a fourth order Runge Kutta scheme. The wavefronts are the same as in Figure 1. The rays however are now replaced by small ray segments. Although no individual rays were traced, the segments are plotted to provide insight into the structure of the ray-field. The number

of ray segments connecting two wave fronts is equal to the number of expansion terms used to calculate the second of the two wave fronts. The number of coefficients increases during propagation.

A problem that may occur is that the length scales of variations of the σ -front may vary greatly over the range of ξ . Especially in regions of large geometrical spreading, the variations on a wavefront may be large for a small range of take-off angles. The sampling density needed to approximate the σ -front adequately is determined by those ranges with the smallest length scales of variations. Since the sampling is homogeneously distributed over the range of ξ — actually the sampling distribution is proportional to the weighting function $W(\xi)$ mentioned in Section 5, as in Gaussian quadrature — this results in oversampling and thus inefficiency in regions of slower variations. This is illustrated by the example of Figures 4 and 5. The model in this example consists simply of two Gaussian shape velocity anomalies. The first anomaly the wavefront meets is fast and causes shadow zone with very large geometrical spreading. In order to maintain enough accuracy to actually see the second anomaly behind the first one, the algorithm needs to use a large amount of expansion terms. This results in severe oversampling in the areas of less geometrical spreading as is seen from the density of ray segments at the sides of the ray ensemble. Figure 5 shows the graphs of the ray variables as functions of the ensemble parameter ξ for the last wavefront in Figure 4. It is clear that the variations in these functions are mostly concentrated in a small region of ξ and thus it is this part that determines the number of coefficients to be used in the spectral expansion. This problem is dealt with in the following two sections.

7 OPTIMAL RAY-FIELD PARAMETERIZATION

In the examples of Section 6 we have used take-off angles at the source as ensemble parameters. It turned out that this was not a very efficient choice, because the variations of the various ray-field variables are not distributed homogeneously over the range of take-off angles. The question is now what parameterization to use in order to obtain maximal efficiency of the expansion technique. The highest efficiency is achieved if the number of expansion terms needed for a certain level of accuracy is minimal. Since the function to be approximated is in fact a vector function, the best configuration is such that each vector component needs approximately the same number of terms to achieve its respective accuracy goal. Another way to put this is that all components of the vector should be comparably smooth. To be able to deal with this analytically, we have to define a smoothness or roughness measure for vector functions. The roughness of single valued function is often measured by an integral over the square of the derivative.

An obvious generalization of this is to define the roughness of a vector function by an integral over a weighted sum of the squared derivatives of all components.

In a formal sense this is realized by defining a metric, or norm, in the vector space from which the function is drawn. In our case, the vector space is the phase space, and the metric may be defined by

$$dl^2 = \langle d\mathbf{v}, d\mathbf{v} \rangle_A = d\mathbf{v} \cdot \mathbf{A} \cdot d\mathbf{v}, \quad (16)$$

where $d\mathbf{v}$ is a differential in phase space and \mathbf{A} is a positive definite matrix containing weights. For a one parameter curve $\mathbf{v}(\gamma)$ in phase space this metric defines a corresponding *metric derivative* by

$$\left(\frac{dl}{d\gamma} \right)^2 = \left\langle \frac{d\mathbf{v}}{d\gamma}, \frac{d\mathbf{v}}{d\gamma} \right\rangle_A. \quad (17)$$

The roughness measure R for such a one parameter curve in phase space may then be defined as

$$R = \int_{\gamma_0}^{\gamma_1} \left(\frac{dl}{d\gamma} \right)^2 d\gamma. \quad (18)$$

A proper definition of the phase space metric would be such that the parameterization γ that minimizes the roughness R , also minimizes the number of expansion terms needed for any component of \mathbf{v} . Since the optimal metric will probably be different for each situation and cannot be determined without extensive calculations, the proper thing to do is to define a simple template metric which is adequate for most circumstances, and which may be adapted to specific situations by some rule-of-thumb. The definition of a metric in phase space implies the summation of coordinate and slowness terms, which have a different physical meaning and hence different ranges of values. In order to compensate this we need at least one degree of freedom in the simplified metric. We propose to define the weight matrix by

$$\mathbf{A} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \alpha \mathbf{I} \end{pmatrix}, \quad (19)$$

with α , the *phase space geometrization factor*, the desired degree of freedom. This yields the metric

$$dl^2 = \langle d\mathbf{v}, d\mathbf{v} \rangle_A = d\mathbf{r} \cdot d\mathbf{r} + \alpha d\mathbf{p} \cdot d\mathbf{p}. \quad (20)$$

The problem is now to find the parameterization which minimizes the roughness of a σ -front. To find it, it is important to recognize the following two facts. First, the smoothness of the Lagrangian manifold in phase space ensures us that for any non-degenerate parameterization γ , the metric derivative $dl/d\gamma$ is strictly positive. Second, the integral of this metric derivative is equal to the length of the σ -front in phase space corresponding to the chosen metric, and hence is independent of the actual parameterization. Together these facts allow us to state that the parameterization we are looking for is the one which renders the metric derivative constant

along the σ -front:

$$\frac{dl}{d\gamma} = \text{constant} = C(\sigma), \quad (21)$$

which is shown by means of the calculus of variations (Appendix B).

Although we now know how to choose the ensemble parameterization for maximum smoothness, the real problem is how to achieve this parameterization in practice. Suppose that the criterion (21) is met for one instance of σ , then simply using the system (8) to propagate to the next value of σ will instantly violate it. In order to maintain optimal parameterization throughout the ray-field integration a continuous reparameterization formalism is presented in Section 8.

8 CONTINUOUS REPARAMETERIZATION

Since we are tracing an ensemble of rays, we know for each value of σ not only the derivative along the ray ($\partial\mathbf{v}/\partial\sigma$), but also the derivative along the σ -front ($\partial\mathbf{v}/\partial\xi$). This makes it possible to integrate the ray-field not only along the rays itself, but along more general paths. This is accomplished by adding an extra term to the ray equations which is proportional to the derivative along the σ -front. In essence this implies a reparameterization of the ray-field, which is represented by the new symbol $\tilde{\mathbf{v}}$:

$$\tilde{\mathbf{v}}(\lambda, \gamma) = \mathbf{v}(\sigma(\lambda, \gamma), \xi(\lambda, \gamma)). \quad (22)$$

The new parameters λ and γ may be compared to σ and ξ respectively. Lines of constant λ parameterize what we will still call σ -fronts, while lines of constant γ do not correspond to rays anymore, since the γ -dependence of $\tilde{\mathbf{v}}$ is basically a reparameterization of the ξ -dependence of \mathbf{v} . For an arbitrary function $f(\lambda, \gamma)$ we may now write

$$\frac{\partial \tilde{\mathbf{v}}}{\partial \lambda} = \mathbf{F}(\mathbf{v}) + f(\lambda, \gamma) \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \quad (23)$$

in which we \mathbf{v} now depends on λ and γ as in the right hand side of (22). Equation (23) may be used as a basis for an expansion approach as in Section 4. Appendix D contains a more formal derivation of (23).

The trick is now to choose $f(\lambda, \gamma)$ in (23) in such a way that for the ray-field solution equation (21) holds for every value of λ . To find the proper constraint on $f(\lambda, \gamma)$ we require that:

$$\frac{d}{d\lambda} \left(\frac{dl}{d\gamma} \right) = D(\lambda), \quad (24)$$

where the value of $D(\lambda)$ is the derivative of $C(\lambda)$, which in turn is the equivalent to $C(\sigma)$ from equation (21). Hence the meaning of $D(\lambda)$ is the derivative of the length of the σ -front with λ . Considering

$$\frac{\partial}{\partial \lambda} \left\langle \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma} \right\rangle_A = 2 \left\langle \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \frac{\partial^2 \tilde{\mathbf{v}}}{\partial \gamma \partial \lambda} \right\rangle_A, \quad (25)$$

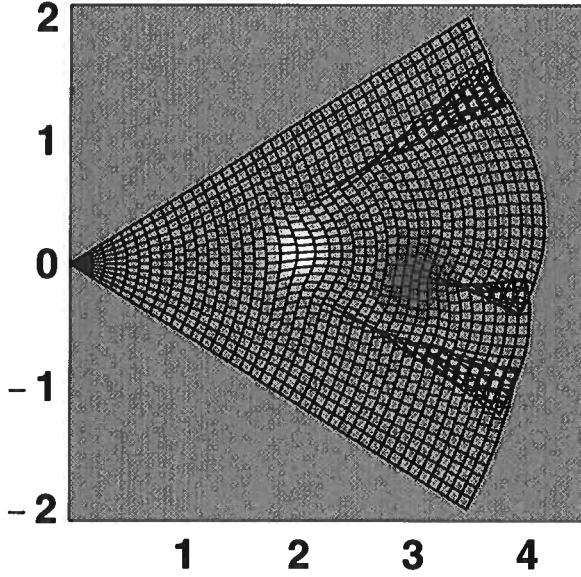


Figure 6. The same ray-field as in Figure 4, now using the continuous reparameterization formalism. The ray-field is now homogeneously sampled.

for any choice of metric, we can derive using (17) and (23)

$$\begin{aligned} \frac{\partial}{\partial \lambda} \left(\frac{dl}{d\gamma} \right) &= \left[\left\langle \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \frac{\partial \mathbf{F}(\tilde{\mathbf{v}})}{\partial \gamma} \right\rangle_A \right. \\ &+ \left. f(\lambda, \gamma) \left\langle \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \frac{\partial^2 \tilde{\mathbf{v}}}{\partial \gamma^2} \right\rangle_A + \left(\frac{\partial f(\lambda, \gamma)}{\partial \gamma} \right) \left(\frac{dl}{d\gamma} \right)^2 \right] \left(\frac{dl}{d\gamma} \right)^{-1}. \end{aligned} \quad (26)$$

Since the magnitude of $d\tilde{\mathbf{v}}/d\gamma$ is constant, the second term in the right hand side vanishes. This is easily verified if we recognize

$$\left\langle \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \frac{\partial^2 \tilde{\mathbf{v}}}{\partial \gamma^2} \right\rangle_A = \left(\frac{dl}{d\gamma} \right) \frac{\partial}{\partial \gamma} \left(\frac{dl}{d\gamma} \right). \quad (27)$$

Together, equations (24) and (26) yield an expression for the derivative of $f(\lambda, \gamma)$, which should be satisfied everywhere to achieve optimal parameterization:

$$\frac{\partial f(\lambda, \gamma)}{\partial \gamma} = \frac{D(\lambda)}{C(\lambda)} - \left\langle \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \frac{\partial \mathbf{F}(\tilde{\mathbf{v}})}{\partial \gamma} \right\rangle_A C(\lambda)^{-2}. \quad (28)$$

Hence $f(\lambda, \gamma)$ is determined except for two constants which can be used to specify $f(\lambda, \gamma) = 0$ at the boundaries of the ensemble.

Although the right hand side of (23) is more expensive to calculate than the original one (8), the new method is more efficient in many cases, owing to the need for less expansion terms. With respect to the wave front construction methods there are two obvious advantages. First, the insertion of rays is a cumbersome practice which takes much numerical overhead. This

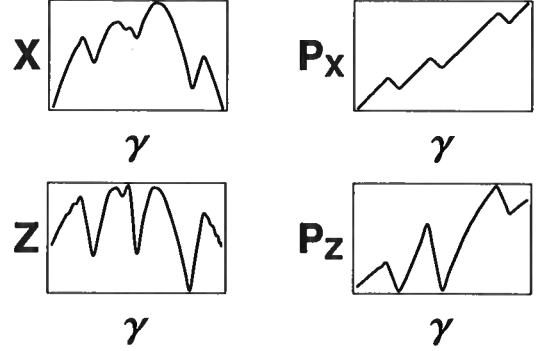


Figure 7. Graphs of the ray-field variables as a function of ensemble parameter γ . The graphs correspond to the last wavefront plotted in Figure 6, and are much smoother than the corresponding ones in Figure 5

new method provides the same effect by simply using more coefficients. Second, the insertion of a ray happens at the moment that the distance between two rays exceeds a critical value. After insertion, however, the distance is halved, and a situation of oversampling occurs. This means that for the greater part of the integration the wave front is highly oversampled. In the continuous case the number of coefficients can be chosen closer to the critical value, and thus be more efficient in that sense. This adds up to the fact that the rapid convergence properties of the spectral expansions allow for a smaller number of coefficients anyway. The continuous reparameterization method is illustrated in Figures 6 and 7. These Figures show the same model as Figures 4 and 5 from Section 6, but now computed using the reparameterization approach. It is obvious both from the ray-field plot and from the graphs that the reparameterization does a good job in reducing the number of expansion terms needed.

9 RAY-FIELD PROJECTION

The integration of the ray tracing system (23) yields ray-related variables such as position, slowness, amplitude, travel time as a function of the independent parameters (λ, γ) . Finding out which rays arrive at a certain grid-position \mathbf{r}^* means solving the non-linear system

$$\mathbf{r}(\lambda, \gamma) = \mathbf{r}^*. \quad (29)$$

There may be multiple solutions, each corresponding to a distinct arrival. The total number of solutions is unknown a priori. This means that in general finding all solutions in such a system is an exhaustive search. This problem may be attacked in three ways.

The first way and conceptually simplest way is to divide the ray field into cells in a way similar to (Lambaré *et al.*, 1996), followed by linear interpolation inside the cells. Another way is to locate the caustics in the

ray field. The caustics, expressed in terms of the ray parameters, separate different branches of the ray-field, each of which has a single solution to the projection algorithm. Finally, we may use the fact that the total number of real and complex solutions to a polynomial system of equations is known a priori. The real solutions correspond to the ray-geometric arrivals. Since we use Chebyshev polynomials to expand the ray-field, we are able to find all solutions. For example if one of the coordinates is used as independent parameter λ , each arrival is found by solving numerically a single polynomial equation. If another independent parameter is used, its dependence should also be fitted by a polynomial, which then yields a system of two bivariate polynomial equations. Similarly in 3D this gives a system of either two or three polynomial equations in as many variables. Although solving a system of polynomial equations is numerically demanding, the work is greatly reduced by using the solutions of one grid point as starting values for next. The polynomial system for neighboring grid points is only slightly different, which allows the use of perturbation methods. Since the projection is not central to this paper we present this approach in a future publication.

10 CONCLUSION

A new method for calculating ray-fields in smooth media was developed. The method is based on the observation that in these media ray variables such as position, slowness and travel time are smooth functions of the ray parameters. The dependence of the rays on the initial conditions is approximated using a pseudo-spectral expansion in terms of Chebyshev polynomials. The smoothness of the functions guarantees exponential convergence of the expansion and thus a relatively low number of evaluations of the ray equations. The result of a calculation is a continuous analytic representation of the ray-field which may subsequently be used to project ray information onto a grid defined in the medium, to generate tables of possibly multi-valued travel times and amplitudes for use in imaging and source location algorithms.

In order to overcome difficulties of the method related to variations in geometrical spreading over the range of initial conditions a new ray-field parameterization was conceived. This parameterization allows a more efficient calculation of the ray field and its projections by abandoning the ray itself as the basis of the expansion.

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REFERENCES

- Bleistein, Norman. 1984. *Mathematical methods for wave phenomena*. Academic Press, Inc.
- Boyd, J. P. 2000. *Chebyshev & Fourier Spectral methods*. Mineola, New York: Dover Publications, Inc.
- Fornberg, Bengt. 1996. *A practical guide to pseudospectral methods*. Cambridge University Press.
- Geoltrain, Sébastien, & Brac, Jean. 1993. Can we image complex structures with first-arrival traveltimes? *Geophysics*, **58**(4), 564–575.
- Goldstein, Herbert. 1980. *Classical Mechanics*. Addison-Wesley.
- Guillemin, Victor, & Sternberg, Shlomo. 1977. *Geometric Asymptotics*. Mathematical Surveys. Providence, Rhode Island: American Mathematical Society.
- Hanyga, Andrzej. 1984. Dynamic ray tracing on Lagrangian manifolds. *Geophys. J. R. Astr. Soc.*, **79**, 51–63.
- Kendall, J-M., & Thomson, C. J. 1993. Maslov ray summation, pseudo-caustics, Lagrangian equivalence and transient seismic waveforms. *Geophys. J. Int.*, **113**, 186–214.
- Lambaré, G., Lucio, P., & Hanyga, A. 1996. Two-dimensional multivalued traveltimes and amplitude maps by uniform sampling of a ray field. *Geophys. J. Int.*, **125**, 584–598.
- Lanczos, Cornelius. 1986. *The variational principles of mechanics*. Mineola, New York: Dover Publications, Inc.
- Press, William H., Teukolsky, Saul A., Vetterling, William T., & Flannery, Brian P. 1992. *Numerical Recipes in C*. second edn. Cambridge University Press.
- Červený, V. 2001. *Seismic ray theory*. Cambridge University Press.
- Vinje, Vetle, Iversen, Einar, & Gjøstøl, Håvar. 1993. Traveltime and amplitude estimation using wavefront construction. *Geophysics*, **58**, 1157–1166.

APPENDIX A: HAMILTONIAN SYSTEM FOR FLOW PARAMETER x

We derive a Hamiltonian system which uses one of the independent coordinates as the independent parameter along the ray. We denote by $\tilde{\mathbf{r}}$ the $N - 1$ -dimensional position vector, which is equivalent to \mathbf{r} , but with the one component that we want to use as independent parameter dropped. In a similar way we define the corresponding slowness vector $\tilde{\mathbf{p}}$. The desired independent parameter is called x . The Hamiltonian may in general be interpreted as minus the canonical momentum (read slowness in the ray-context) associated with the independent parameter (Lanczos, 1986; Goldstein, 1980). This means that we must choose:

$$\mathcal{H}_x(\tilde{\mathbf{r}}, \tilde{\mathbf{p}}) = -\sqrt{u^2(x, \tilde{\mathbf{r}}) - \tilde{\mathbf{p}} \cdot \tilde{\mathbf{p}}}, \quad (\text{A1})$$

which gives the ray equations:

$$\frac{d\tilde{\mathbf{r}}}{dx} = -\frac{\tilde{\mathbf{p}}}{\mathcal{H}_x}, \quad \frac{d\tilde{\mathbf{p}}}{dx} = -\frac{u\nabla_{\tilde{\mathbf{r}}}u}{\mathcal{H}_x}, \quad \frac{dT}{dx} = -\frac{u^2}{\mathcal{H}_x}. \quad (\text{A2})$$

APPENDIX B: OPTIMAL PARAMETERIZATION

For a general function $f(\xi)$, which increases monotonously between ξ_0 and ξ_1 , we want to find a reparameterization in terms of γ ($\gamma_0 \leq \gamma \leq \gamma_1$) such that the roughness condition of equation (18) is minimized. We write

$$\bar{f}(\gamma) = f(\xi(\gamma)), \quad (\text{B1})$$

with $\bar{f}(\gamma_0) = f(\xi_0)$ and $\bar{f}(\gamma_1) = f(\xi_1)$. For the roughness integral we get

$$R_\gamma = \int_{\gamma_0}^{\gamma_1} (f'(\xi)\xi'(\gamma))^2 d\gamma. \quad (\text{B2})$$

Using calculus of variations (e.g. (Lanczos, 1986)) the requirement $\delta R_\gamma = 0$ gives the Euler-Lagrange equation

$$\frac{d}{d\gamma} (f'(\xi)\xi'(\gamma)) = \frac{d\bar{f}'(\gamma)}{d\gamma} = 0. \quad (\text{B3})$$

This shows that the derivative of the function in the new parameterization is constant. The constant is determined by the prescribed values of the functions on the boundaries of the domain.

APPENDIX C: DETERMINATION OF PHASE SPACE METRIC

The purpose of the phase space metric and the phase space geometrization factor α (20) is to be able to relate variations in slowness to variations in spatial coordinates. Comparable smoothness of these quantities along the range of γ may only be achieved if the metric is more or less equally sensitive to variations in both.

We want to choose α in such a way that both terms on the right hand side of (20) are of similar scale. The right tool to find a rule-of-thumb to determine α is scale analysis. We approximate the slowness of the medium $u(\mathbf{r})$ by a constant U , and the gradient of the slowness by

$$\nabla u(\mathbf{r}) \approx \frac{\delta U}{L_U}, \quad (\text{C1})$$

where δU is representative for the variations in the slowness, and L_U the corresponding length scale. Now first consider the case where all space coordinates and slowness components are dependent variables. The square of the metric derivative is then given by

$$\left(\frac{dl}{d\gamma}\right)^2 = \frac{d\mathbf{r}}{d\gamma} \cdot \frac{d\mathbf{r}}{d\gamma} + \alpha \frac{d\mathbf{p}}{d\gamma} \cdot \frac{d\mathbf{p}}{d\gamma}. \quad (\text{C2})$$

The slowness may be represented by

$$\mathbf{p} = u(\mathbf{r})\hat{\mathbf{n}}, \quad (\text{C3})$$

where we disregard any dependence on σ , and

$$\hat{\mathbf{n}}(\gamma) = \begin{pmatrix} \cos \theta(\gamma) \\ \sin \theta(\gamma) \end{pmatrix}, \quad (\text{C4})$$

with $\theta(\gamma)$ the angle of \mathbf{p} with the x -axis. This gives

$$\frac{d\mathbf{p}}{d\gamma} \cdot \frac{d\mathbf{p}}{d\gamma} = \left(\nabla u(\mathbf{r}) \cdot \frac{d\mathbf{r}}{d\gamma}\right)^2 + u(\mathbf{r})^2 \left(\frac{d\theta}{d\gamma}\right)^2. \quad (\text{C5})$$

For the scale analysis we now substitute each derivative to γ by an estimate as in the case of \mathbf{r} :

$$\left|\frac{d\mathbf{r}}{d\gamma}\right| \approx \frac{\Delta r}{\Delta \gamma}, \quad (\text{C6})$$

which gives

$$\left(\frac{dl}{d\gamma}\right)^2 \approx \left(\frac{\Delta r}{\Delta \gamma}\right)^2 + \alpha \left[\left(\frac{\delta U}{L_U} \frac{\Delta r}{\Delta \gamma}\right)^2 + U^2 \left(\frac{\Delta \theta}{\Delta \gamma}\right)^2 \right]. \quad (\text{C7})$$

A value for α is now found by equating the first and the second term of the right hand side:

$$\begin{aligned} \alpha &\approx \left(\frac{\Delta r}{\Delta \gamma}\right)^2 \left[\left(\frac{\delta U}{L_U} \frac{\Delta r}{\Delta \gamma}\right)^2 + U^2 \left(\frac{\Delta \theta}{\Delta \gamma}\right)^2 \right]^{-1} \\ &= \left(\frac{\delta U^2}{L_U^2} + \frac{U^2}{R^2}\right)^{-1}, \end{aligned} \quad (\text{C8})$$

where R , defined as

$$R = \frac{\Delta r}{\Delta \theta}, \quad (\text{C9})$$

is a representative value for the radius of curvature of the wave fronts. It depends on the medium and the initial conditions which of the terms in (C8) dominates.

If one of the space coordinates is used as independent parameter the case is slightly different. If x is independent for example, and y is the dependent variable with slowness component $u(\mathbf{r}) \sin \theta$, the metric turns out to be

$$\left(\frac{dl}{d\gamma}\right)^2 = \left(\frac{dy}{d\gamma}\right)^2 + \alpha \left(\frac{du(\mathbf{r})}{dy} \frac{dy}{d\gamma} \sin \theta + u(\mathbf{r}) \cos \theta \frac{d\theta}{d\gamma}\right)^2. \quad (\text{C10})$$

This yields for α :

$$\alpha \approx \left(\frac{\delta U}{L_U} \sin \theta + \frac{U}{R} \cos \theta\right)^{-2}, \quad (\text{C11})$$

where it should be noted that θ is often small, to allow x to be used as an independent parameter. The most difficult part of these estimations of α is the a priori determination of a characteristic radius of curvature.

APPENDIX D: DERIVATION OF EQUATION (23)

We will now derive equation (23) in a more formal way by considering the change of parameterization from

(σ, ξ) to (λ, γ) . The total differential for the new parameterization $\tilde{\mathbf{v}}$ in terms of the old \mathbf{v} gives:

$$\begin{aligned} d\tilde{\mathbf{v}} &= \left[\left(\frac{\partial \mathbf{v}}{\partial \sigma} \right) \left(\frac{\partial \sigma}{\partial \lambda} \right) + \left(\frac{\partial \mathbf{v}}{\partial \xi} \right) \left(\frac{\partial \xi}{\partial \lambda} \right) \right] d\lambda \\ &+ \left[\left(\frac{\partial \mathbf{v}}{\partial \sigma} \right) \left(\frac{\partial \sigma}{\partial \gamma} \right) + \left(\frac{\partial \mathbf{v}}{\partial \xi} \right) \left(\frac{\partial \xi}{\partial \gamma} \right) \right] d\gamma. \end{aligned} \quad (\text{D1})$$

Since we have no reason to reparameterize in the direction along the rays, we will now choose

$$\frac{\partial \sigma}{\partial \lambda} = 1, \quad \text{and} \quad \frac{\partial \sigma}{\partial \gamma} = 0, \quad (\text{D2})$$

such that λ is equivalent to σ , and lines of constant λ will coincide with σ -fronts. Combining equations (D1) and (8) we get

$$\frac{\partial \tilde{\mathbf{v}}}{\partial \lambda} = \mathbf{F}(\mathbf{v}) + \left(\frac{\partial \mathbf{v}}{\partial \xi} \right) \left(\frac{\partial \xi}{\partial \lambda} \right), \quad \text{and} \quad (\text{D3})$$

$$\frac{\partial \tilde{\mathbf{v}}}{\partial \gamma} = \left(\frac{\partial \mathbf{v}}{\partial \xi} \right) \left(\frac{\partial \xi}{\partial \gamma} \right). \quad (\text{D4})$$

To be able to compute the ray-field in its new parameterization we eliminate the partial derivative to ξ in equation (D3), using (D4):

$$\frac{\partial \tilde{\mathbf{v}}}{\partial \lambda} = \mathbf{F}(\mathbf{v}) + \left(\frac{\partial \xi}{\partial \gamma} \right)^{-1} \left(\frac{\partial \xi}{\partial \lambda} \right) \frac{\partial \tilde{\mathbf{v}}}{\partial \gamma}, \quad (\text{D5})$$

and since we are still free to choose how ξ depends on λ and γ , we may use

$$f(\lambda, \gamma) = \left(\frac{\partial \xi}{\partial \gamma} \right)^{-1} \left(\frac{\partial \xi}{\partial \lambda} \right), \quad (\text{D6})$$

to get equation (23).