Propagation of Discontinuities in Wave Fields

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Abstract

Ray methods play an important role in the investigation and computation of discontinuities in waves. Tracing amplitudes along rays leads to difficulties at caustics. Here a numerically feasible method is proposed to overcome those problems. It is applicable to transient waves directly, and it allows explicit time dependencies in the data. The method derives from known results in the theory of linear partial differential equations.

Introduction

In seismics high-frequency waves are used to investigate the structure of the earth's interior - or at least part of it. Seismograms are recordings of such waves.

The propagation of high-frequency waves is governed by the laws of geometrical acoustics: disturbances propagate along rays. It is a major task for mathematical physics to understand the relationship between rays and waves in detail.

This paper relates to a topic which is called 'dynamic ray tracing' in the seismics literature. Here one is interested in obtaining computationally feasible procedures for tracing rays and, along them, the ray data which are relevant for computing the wave fields themselves: wavefront curvatures and amplitudes.

Only the interior (dynamic) ray tracing in the absence of interfaces is treated here. The main emphasis is on techniques for handling caustics correctly. Also the inversion problem is not attacked here. Of course, it is hoped that dynamic ray tracing in a background or reference model may turn out to be useful for the inverse problem.

The theoretical basis for ray tracing as developed here is the modern theory of linear partial differential equations. This allows a fresh view on known results on dynamic ray tracing. Furthermore, it becomes possible to extend the scope of some of these results. An example for this is the possibility to deal with transient waves directly.

Since the methods underlying the approach sketched here may be unfamiliar to geophysicists this article is given an expository style.

Discontinuous Waves

For transient waves, i.e. waves defined on the space-time domain as opposed to the space-frequency domain, high-frequency content corresponds – via the Fourier transform – to discontinuities, e.g. jumps or spikes (Dirac deltas).

Waves are solutions to hyperbolic partial differential equations. For simplicity, consider the standard wave equation in free space $\mathbb{R}_t \times \mathbb{R}^3_x$,

$$\Box u := u_{tt} - c(x)^2 \Delta u = 0.$$

Here $c > 0$ is the wavespeed. Let h denote the Heaviside unit step function on the real line. To solve $\Box u = 0$ one can try an ansatz

$$u(t,x) = a(t,x)h(t - \phi(x)) + \ldots.$$

for a wave with a jump discontinuity across the wavefront $t = \phi$. This ansatz can lead to a non-trivial approximate solution for $\Box u = 0$ only when the phase ϕ solves the eiconal equation,

$$c \mid \nabla \phi \mid = 1,$$

and when the amplitude a solves the transport equations,

$$\dot{a} + c^2 \Delta \phi \, a/2 = 0.$$

The latter are ordinary differential equations for the restrictions of a to the rays $x(t)$, $\dot{x} = c^2 \nabla \phi$.

The geometrical acoustics ansatz does not give exact solutions for the wave equation. To achieve this the ansatz has to be corrected with a solution to an inhomogeneous wave equation. Here other solution methods must be used. Courant and Lax [4] were the first to employ the L^2 existence and regularity theory for linear hyperbolic partial differential equations for this purpose. The backbone of this theory are energy estimates combined with functional analysis [7,13]. This solution method is often non-constructive. However it allows to prove rigorously statements of the following type:

> Let ϕ and a solve the eiconal and the transport equations, respectively. Then there is a continuous function v such that

$$u(t,x) = a(t,x)h(t - \phi(x)) + v(t,x)$$

solves $\Box u = 0$ exactly.

v has no jumps. Therefore the discontinuities in u are completely given by ϕ and a. Furthermore, one can see that discontinuities propagate along rays. Results of this kind justify the geometrical acoustics approximation. Therefore it is reasonable to restrict attention to the solution of the eiconal and transport equations. This will be done in the following.

Courant and Lax [4] proved a result of the above type for initial value problems for hyperbolic systems. When contrasted with other methods for obtaining exact solutions, e.g. separation of variables or Weyl-Sommerfeld integral, the Courant-Lax approach has a significant advantage in its generality and flexibility. For example, it is not necessary to make any assumptions on the wave speed except for its smoothness.

The modern development of these ideas takes place in the framework of microlocal analysis. The techniques of microlocal analysis allow one to think of linear partial differential equations as defined on phase space (microlocal = local in the cotangent bundle or phase space). A basic reference for this is Hörmander's four-volume monograph [12].

Ray Tracing I

The eiconal equation is a first order nonlinear partial differential equation. Classical Hamilton-Jacobi theory explains how it can be solved by solving a system of ordinary differential equations,

$$\dot{x} = \partial H/\partial\xi \text{ and } \dot{\xi} = -\partial H/\partial x.$$

Here $H = c(x)\,|\xi\,|$ is the Hamilton function, defined on phase space $\mathbb{R}^3_x \times \mathbb{R}^3_\xi$. x and ξ are the position and momentum vectors, respectively. The solutions to Hamilton's canonical equations given above are called bicharacteristics or rays in phase space. The basic relation between these and the eiconal equation is: Rays hitting the graph of $\nabla\phi$, i.e. the manifold

$$\Lambda_\phi = \{(x, \nabla\phi(x)\},$$

are tangent to it. Therefore Λ_ϕ is a union of rays. Since $\dot{\phi} = 1$ along a ray the phase ϕ itself is obtained as traveltime.

To set up the transport equations for the amplitude, one needs to know the second derivatives of the phase (traveltime) along rays. The evolution of the Hessian of the phase, $W = \nabla^2\phi$, is governed by a Riccati equation ,

$$\dot{W} + WW + C = 0.$$

Here C is a 3×3 matrix depending only on the wavespeed c and its first and second derivatives. The differential equation for W follows from differentiation of the eiconal equation.

The geometrical meaning of the symmetric 3×3 -matrix W is that of a wavefront curvature tensor. Below a different interpretation for W will be more important. W defines the tangent space of the manifold Λ_ϕ: (x, ξ) is a tangent direction to Λ_ϕ if and only if $\xi = Wx$. This follows by differentiating the equations defining Λ_ϕ.

W enters the transport equations through its trace

$$\Delta\phi = \text{trace } (\nabla^2\phi).$$

This term causes the geometrical spreading and focussing phenomena.

Caustics

The dynamic ray tracing method sketched above is of course well-known. It is also well-known that the development of caustics leads to a break-down in this method. Caustics show up in a multivaluedness of the phase ϕ and in the occurrence of poles in the wavefront curvature $W(t)$. In particular, the eiconal equation is not globally solvable when caustics are present.

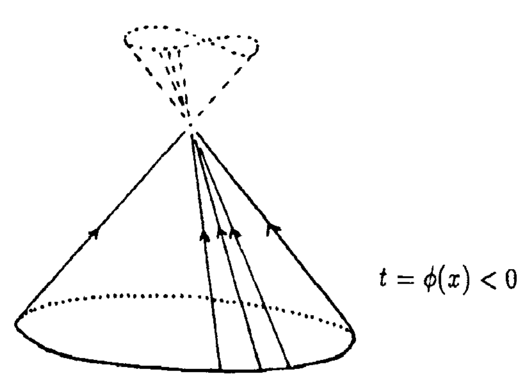
Example. In a space-time setting with $c = 1$ one may take a solution u to the wave equation which has a discontinuity on a light-cone,

$$t = -|x| < 0,$$

with tip at the origin (see figure). Here $\phi = -|x|$. The rays are the straight lines given by

$$x(t) = t\xi \text{ for } t < 0.$$

Here ξ is a constant vector with $|\xi| = 1$. As $t \to 0-$ the wavefront curvatures W , $\Delta\phi$ and the amplitudes a blow up like t^{-1}.



The geometrical acoustics constructions mentioned above lead to a solution

$$u(t,x) = t^{-1}h(t+|x|) + v(t,x)$$

of the wave equation in $t < 0$ with a continuous remainder v. How does the solution u continue from $t < 0$ to $t \geq 0$? Rays can be traced across the caustic at the space-time origin. Is a geometrical acoustics approximation valid also in $t > 0$?

A neat and general solution to the caustics problems was given by Maslov [14]. Here is a very rough outline of his ideas. The concept of a Lagrangian manifold is fundamental to his approach. Lagrangian manifolds are submanifolds of phase space of dimension 3 on which the symplectic 2-form $d\xi_j \wedge dx_j$ vanishes. The Λ_ϕ's are particular examples of Lagrangian manifolds. The eiconal equation is rewritten as: $H = 1$ on Λ_ϕ, and generalized to:

$$H = 1 \text{ on } \Lambda$$

with Lagrangian manifolds, Λ, allowed as solutions. A solution Λ is obtained with a generalization of Hamilton-Jacobi theory as a union of rays. Since rays can be continued indefinitely there is no obstruction to solving the eiconal equation in this generalized sense. Amplitudes a and transport equations are defined up on Λ and not down in x-space. With solutions Λ and a of the generalized eiconal and transport equations, respectively, one can also associate an (approximate) solution u to the wave equation. This however requires that a satisfies a special transformation law on Λ under change of coordinates. This law reflects the well-known phase shift phenomenon occurring after passage through a caustic. Quite generally, problems with caustics are overcome in phase space by choosing appropriate canonical (= symplectic) coordinates. In x-space caustics occur precisely at points where the projection from Λ down to $\mathbb{R}^3_x$ drops rank.

The mathematical foundation of Maslov's method was secured largely by Arnold [1] and Hörmander [11]. Maslov's approach is known in the seismics literature [2,9].

Linearized Lagrangian manifolds

For dynamic ray tracing it is necessary to replace the wavefront curvatures W by objects which are also defined at caustics. Such objects are the tangent spaces λ of a Lagrangian manifold Λ solving the eiconal equation.

The tangent space λ to Λ at a given point on Λ is the 3-dimensional linear subspace of $\mathbb{R}^3_x \times \mathbb{R}^3_\xi$ consisting of all tangent directions to Λ at that point. λ can be represented by a system of linear equations,

$$\lambda : \; y + L\eta = 0.$$

Here L is a symmetric 3×3 - matrix. (y, η) are suitable canonical coordinates defined by a symmetric 3×3-matrix T,

$$(y, \eta) = (x, \xi + Tx).$$

Here and in the following it is not necessary for the dimension to be 3. Any dimension $n \geq 1$ is allowed, e.g. $n = 4$ for space-time.

As noted earlier the wavefront curvatures W – when existing – define the tangent spaces λ to $\Lambda = \Lambda_\phi$. If W^{-1} exists the representation above holds with $L = W^{-1}$ and $T = 0$. If W^{-1} does not exist $T \neq 0$ has to be chosen suitably.

Given a tangent space $\lambda \subset \mathbb{R}^{2n}$ to a Lagrangian manifold one would like to find symmetric $n \times n$ - matrices L and T representing λ. In addition, one would like L and T to have moderate sizes. A stable algorithm for computing L and T is described and analysed in [8]. The algorithm employs Householder reductions, and it is based on facts from symplectic linear algebra.

It follows from Maslov's theory that the amplitude a must be multiplied with a factor,

$$|\det(M)|^{-1/2} \exp(\pi i \ \mathrm{sign}(M)/4),$$

$i = \sqrt{-1}$, when the representing matrices L and T are changed. Here M is a symmetric $2n \times 2n$ - matrix which can easily be assembled from the old and new L and T, see e.g. [12, vol. III 21.6]. This factor is called the Maslov factor. It is readily computed. In fact, there are stable algorithms available for computing the determinant and the signature of symmetric matrices.

Ray Tracing II

Now the ordinary differential equations for dynamic ray tracing of transient waves can be stated. These are valid for a very general class of linear partial differential operators, called operators of real principal type. The ray equations are derived from formulas and theorems proved by Duistermaat and Hörmander [6] in their theories on Fourier integral operators and on the propagation of singularities in solutions to equations of real principal type. See also [12, vol. IV chapters 25 and 26] for a more recent presentation.

The ray equations depend on the principal symbol p and the subprincipal symbol p_{sub} of the operators. Both symbols are defined on phase space over space-time $\mathbb{R}^4_x \times \mathbb{R}^4_\xi$, e.g. for the wave operator $\Box$,

$$p = \xi_0^2 - c(x)^2(\xi_1^2 + \xi_2^2 + \xi_3^2).$$

x_0 is the time coordinate. p_{sub} corresponds to lower order terms in the operator.

Rays (= bicharacteristics) are curves $(x(s), \xi(s))$ in phase space with $\xi \neq 0$ satisfying $p(x(s), \xi(s)) = 0$,

$$\dot{x} = \partial p / \partial \xi \text{ and } \dot{\xi} = -\partial p / \partial x.$$

Here the ray parameter s need not agree with time.

The tangent spaces $\lambda(s)$ along a given ray in a Lagrangian manifold are represented with symmetric 4 × 4 - matrices $L(s)$ and T,

$$y + L(s)\eta = 0 \text{ where } (y, \eta) = (x, \xi + Tx).$$

T does not depend on s. $L(s)$ satisfies the matrix ordinary differential equation

$$\dot{L} + Lp''_{yy}L - p''_{\eta y}L - Lp''_{y\eta} + p''_{\eta\eta} = 0.$$

Here the second derivatives of the principal symbol taken at points on the underlying (axial) ray enter.

Given the axial ray and the curve of tangent spaces the transport equation for the amplitude a along this ray is the linear ordinary differential equation

$$\dot{a} + \text{ trace } (p''_{yy}L - p''_{y\eta})\, a/2 + i\, p_{sub}\, a = 0.$$

p_{sub} is often purely imaginary. It contains the terms which can cause the damping of amplitudes.

Like the differential equation for W stated earlier the differential equation for L is of Riccati-type. Therefore L can – and in general will – blow up. But now this blow-up is no obstacle to dynamic ray tracing. In fact, when $L(s)$ becomes large one can simply pass to new moderately sized representors $L(s)$ and T for $\lambda(s)$ with the algorithm mentioned in the previous section. Then the pole will be removed. When such a change is made the amplitude a must also be multiplied with the Maslov factor.

It is important to note that for this method of handling caustics it is not necessary to know the location of caustics in advance. These can be found and handled automatically during ray tracing.

Remark. It may be helpful to look at a situation which is analogous to the above but simpler. $y(x) = \tan x$ solves the initial value problem $y' = 1 + y^2$, $y(0) = 1$. The integration can be carried across the pole at $x = \pi/2$ by changing to the dependent variable $z = 1/y$, i.e. by changing from $\tan x$ to $\cot x$. The differential equation transforms into $z' = -1 - z^2$. Where z blows up one can switch back to $y = 1/z$.

The ray tracing equations stated above have natural generalizations to systems of real principal type, in particular, to the equations of (isotropic) elastodynamics. The amplitudes are vector-valued then. In the transport equations the rotation of polarization is caused by the subprincipal symbol. A derivation of these equations can be given on the basis of computations made by Dencker [5]. It will be given elsewhere.

Remarks

The ray tracing method introduced here can be generalized to include the reflection and refraction of rays, tangent spaces, and amplitudes at interfaces. Because of the space-time setting adopted here there is no problem in dealing with explicit time dependencies in the coefficients (and interfaces).

Hanyga [9,10] has developed dynamic ray tracing on the basis of Maslov theory. In [10] a computer program is described. The appproach outlined here differs considerably from Hanyga's.

The Gaussian beam method is an alternative to ray tracing based on Maslov theory, see Červený et al. [3], and Ralston [15]. Here the poles developing in solutions to the Riccati equations are avoided by passing into the complex plane.

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