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Acoustic ray tracing in complex 3D media

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Abstract

The numerical solution of ray tracing problems in complex 3D media is considered in this paper that reviews some of the work and applications in which the author and his collaborators have been engaged in the past few years. The paper is not a survey but rather tries to point out what are the main issues common to many applications and how we have attacked the problem and implemented computational tools with general applicability to such disparate fields as earthquake seismology, oil prospecting, and non-destructive evaluation of complex mechanical parts.

1 Introduction

Ray tracing provides a way to simulate numerically some aspects of wave propagation. It is not as comprehensive as finite difference or finite element methods, but it is considerably more economical. With its geometrical flavour it is also a more intuitive tool, producing results that are easier to analyze and interpret.

In three dimensional complex media, ray tracing is not as straightforward as it might be in 2D, or in, say, layered 3D media. The complexity of the media may be due to geometry, to general inhomogeinities, or a combination of both. Generally one is interested in tracing many rays, and different applications will require the solution of somewhat different problems. Most often this difference will appear in the boundary or interface conditions.

In order to create a robust, flexible, and efficient tool, capable of solving a variety of problems in different application fields, one needs to consider as part of the problem the issues of model description and acquisition. Once a model structure and parametrization has been decided, then a ray tracing algorithm capable of calculating accurate ray paths and ray amplitudes in such models has to be devised.

For a number of years we have been working on such algorithms, and their implementations in generally usable computer code. The development of user interfaces, interactive graphical input and display of models for a number of different applications has also been an important concern in recent times [1, 3, 6, 11]. We explain in this paper some of the ingredients of one such implementation and briefly indicate some of its applications.

Ray tracing (the geometrical theory of optics) is by no means a novel technique; it certainly goes back to Huygens and probably earlier. In its more modern version has been used as the backbone of an asymptotic theory for wave propagation. What has changed in recent times is that, with the improvement in computing power available, much more ambitious applications are within the reach of interactive computations on desktop workstations or even personal computers.

Although there is some overlap in the approach, we emphasize that we will not be concerned here with ray tracing as used in computer graphics for realistic rendering of 3D scenes.

2 Modeling paradigm

We will consider in this discussion a bounded region of 3D space, say a paralellepiped **P** for simplicity, where our domain of study or "scene" will lie. A mathematical model of this scene is a (usually simplified or idealized) representation of those aspects that are relevant to the physical process to be modeled. In the case of acoustic wave propagation we will be interested in the velocity of propagation of acoustic waves and density at every point in **P**. In the presence of radically different materials, these quantities will have sharp discontinuities. The surfaces separating different materials will be called interfaces and they will represent the spatial locations of the discontinuities of the velocity field. They usually will have intrinsic interest, since sound waves will partially reflect when reaching such discontinuities.

In elastic wave propagation we will also need the velocity of propagation of shear waves, and in anisotropic media many more parameters may be required to completely describe the phenomenon.

A region may be composed of an homogeneous or smoothly varying inhomogeneous material. This is one of the idealizations we were refering to above, and it will be justified if the material properties vary slowly and in a regular way. A smooth representation is in itself a way of filtering high frequency noise and it will be acceptable only if it agrees with the wave lengths and scale of the application. If however, the wavelengths are such that inhomogeneities are seen as irregular, then wave propagation in random media may be the appropriate tool. We will not deal with that situation here. The interested reader can consult [13, 15, 16].

Thus, the general type of scenes that we will consider are those where the modeling region **P** is subdivided into sub-regions of irregular shape, bounded by surface patches, containing either homogeneous or smoothly varying inhomogeneous materials. The bounding surface patches will be either part of the faces of the bounding box **P**, or they will be interfaces between two sharply different materials. We some times refer to these interfaces as strong reflectors, depending on the impedance contrast between the materials on their two sides. From the point of view of geometrical ray tracing, these are the surfaces at which, upon incidence, rays will change direction discontinously, either under reflection or transmission (refraction) modes.

Mathematically we will then consider our scene as being described by two (or more) piecewise smooth functions of three variables, with the discontinuity manifolds explicitly modeled as smooth surfaces, and where some sort of connectivity table indicates which surface patches bound which regions. Derivative discontinuities will be permitted accross the common curves between two adjacent smooth surface patches, thus allowing the modeling of sharp edges. We will insist that a surface patch has only one kind of material on each side. In this way, when a ray traverses (transmit through) an interface patch, there will be an unequivocal rule to indicate which new region the ray is getting into. This simple requirement will make the navigation of a complicated model possible.

A hierarchical, object oriented structure is quite appropriate and convenient to describe models:

```
Points ---> Curve segment ---> Composite curves --->
Surface patches ---> Composite surfaces ---> Regions ---> Model
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As an example we can consider:

Curve segment: {straight line, arc of circle, cubic spline, ...},
which indicates the open ended nature of the data structures.

Basic operations are to be identified and associated with each object type. In this form, object encapsulation will permit the addition of new object instances without affecting the rest of the code.

If the tool created is going to be used by a wide audience to solve real everyday problems, it is mandatory that a modern friendly graphical user interface be devised. This should be application dependent and require from the users the minimum natural input to define their particular problem. In some cases, if the problem domain is very well specified, it will be possible to automate large parts of the model construction (usually the most tedious and error prone part of the process). Some details on implementations for seismic oil exploration and non-destructive ultrasound inspection of nuclear reactors can be found in the references cited in the Introduction.

3 Ray tracing

A ray tracing calculation has two main components. One is purely geometrical: finding the ray path (or paths) with some given characteristics. The second one requires the calculation of the acoustic atenuation of a given signal as it travels through the medium. This amplitude calculation has itself two parts: one purely geometrical (spreading), while the second one requires the evaluation of the partition of energy as the ray reaches a discontinuity in the medium.

The ray path calculation depends on the definition of the task. A simple task may consist of shooting or casting rays from a known position (source), in a given direction, and letting them fly through the medium following some prescribed rules to choose between reflected or transmitted wavefronts (ray signature), until some terminal condition is fulfilled.

A more complicated problem is that of calculating the ray path (or paths) between given source and receiver positions. If the source and receiver positions are coincident, as in the case of a transceiver for pulse-echo applications or the simulation of stacked traces in petroleum exploration, there must be a reflector where the ray incidence is normal. In that case, one can usually halve the amount of computation by tracing only a one way path. Otherwise, if there is an offset between the source and the receiver, the full trajectory needs to be calculated. In the presence of variable velocity, ray bending may provide direct transmission between source and receiver, without needing to resort to reflection.

If we call $\eta = (x(s), y(s), z(s))$ to the vector function describing the ray trajectory parametrized by arc length s, and $\mathbf{w} = u(\eta)\dot{\eta}$, where $u(\eta) = 1/v(\eta)$, and $v(\eta)$ is the velocity of propagation, then the ray equations can be derived either from the Eikonal equation, or by invoking Fermat's principle of minimum time. A convenient form in 3D is:

$$\dot{\eta} = v\,\mathbf{w} \tag{1}$$

$$\dot{\mathbf{w}} = \nabla\, u. \tag{2}$$

This is a system of six first order, nonlinear (as soon as the velocity is nonconstant), ordinary differential equations (ODE's), that is valid within any smooth subregion of the model.

The problems we mentioned above are completely described by adding appropriate initial and/or end conditions:

Shooting: $\eta(0) = \eta_0, \quad \mathbf{w}(0) = \mathbf{w_0},$

Source/receiver: $\eta(0) = \eta_0, \quad \eta(S) = \eta_{\mathbf{end}},$

where S is the total arc length along the ray path (usually unknown).

Additionally, if the ray path encounters material discontinuities, internal boundary conditions will be needed. Generally these will be:

Continuity of the ray path: $\eta(s_i^+) = \eta(s_i^-),$

Snell's law: $\mathbf{w}(s_i^+) = \mathbf{w}(s_i^-) + \{\pm\sqrt{u(s_i^+)^2 - u(s_i^-)^2 + \alpha^2} - \alpha\}\mu(s_i),$

where, s_i^+, s_i^- indicate the incident and transmitted sides of the interface, $\mu(s_i)$ is the normal to the interface at the incidence point, and $\alpha = < \mathbf{w}(s_i^-), \mu(s_i) >$ is proportional to the cosine of the angle between the outgoing ray direction and the normal to the reflector. Finally, the

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+ sign in front of the square root corresponds to transmission, while the − sign indicates reflection. In the latter case, Snell's law simplifies to: $\mathbf{w}(s_i^+) = \mathbf{w}(s_i^-) - 2\alpha\mu(s_i)$.

In the shooting case, the ray path calculation requires the solution of an initial value problem for a system of ODE's with discontinuities at unknown locations. This problem can be solved with conventional numerical methods, augmented to dinamically sense and calculate the intersections with the discontinuity surfaces. The task is somewhat complicated by the fact that as the numerical ray travels through the model it usually does not know which one of potentially many surface patches bounding the current region it will meet next.

The source/receiver case requires the solution of a multipoint boundary value problem for the same system of ODE's and it could be solved, in principle, by using the shooting method, enhanced with a search phase to try to satisfy the end conditions. This is quite effective when it works, but it has been known for a long time that shooting techniques for boundary value problems can fail in fairly simple and commonly found situations.

Thus, we prefer to use the more robust global or "bending" methods, coupled with continuation techniques in order to calculate efficiently families of rays of the same type.

Bending is seismologists lingo for describing the finite difference solution of a multipoint boundary value problem for the ray equations [2, 3, 4, 5, 7, 10, 11] . In a nutshell, a mesh along the ray is postulated in some fashion, and a discretized version of the problem is stated, leading to a coupled system of nonlinear algebraic equations. One can take advantage of the special sparse structure to produce a stable, efficient and robust solver. An initial discrete trajectory is required, and then the nonlinear solver is used to bend it until a good approximation to a minimum time path is produced.

In our implementation for obtaining automatically many related ray paths, we use shooting as a low accuracy initialization procedure, and then we switch to a bending algorithm to obtain a more accurate solution. Mesh refinement and a variable order method is employed to adapt the numerical method automatically to the large variety of problems that can be encountered. Once the algorithm has converged to a source/receiver path, we pick a neighboring receiver and use the converged ray path to initialize the new calculation. This process is called receiver continuation. Other types of continuation are possible and useful in different situations.

Geometrical spreading can be calculated by solving the linearized ray equations with appropriate right hand sides. It turns out that due to the type of ray solver used, a factorized version of the discretized linearized ray equations is available upon a successful ray calculation. This is a bonus stemming from the use of bending methods, and it can be exploited in general to calculate derivatives of the state variables with respect to parameters. This is very useful when ray tracing is used to solve inverse problems [4, 5, 7, 8, 10]. Care should be taken if the ray path traverses a focal point, or any other singularity of the wave fronts (caustics). In those cases, geometrical spreading calculations break down and they have to be enhanced with more sophisticated approximations (shadow zones).

The calculation of reflection/transmission coefficients at interfaces in acoustic media involves basically Zoeppritz formulas and it is reasonably straightforward. In elastic media, the appearance of a second mode of propagation complicates considerably the problem. Shear wave polarization has to be transported through the media, and issues like ray torsion and super-critical reflections leading to phase shifts between SH and SV components must be taken into account.

Finally, in a medium with discontinuities, even if we only allow smooth reflecting surfaces, there will be edges, and maybe point diffractors, where again, standard geometrical optics will break down, and more sophisticated approximations have to be considered in order to calculate diffraction coefficients.

4 Applications

The applications we are most familiar with are in petroleum exploration, general seismology and in the ultrasound inspection of complex mechanical parts.

In petroleum exploration, seismic methods have been used for many years to try to map the interior of the earth, at least at depths of interest to oil production (a few kilometers). Artificial sources, like explosions, vibrator trucks or air guns (off-shore), are used to generate elastic or acoustic energy. Listening devices are placed on the surface of the earth, on wells, or are towed by ships, in order to record the back scattered energy after it has traveled through the earth. The idea is that these signals contain information on the material properties of the part of the earth they have visited. 3D realistic geology can be very complex, and the ability to deal with unconformities, like faults, pinched-out layers, salt diapirs with overhangs, folds, and overthrusts, is quite fundamental. For a long time the application of these techniques was limited to 2D simple geometries, and more recently to 3D curved layered media. Today it is possible to represent and construct much more complicated models, and thus more sophisticated ray tracing techniques have become necessary.

A modern 3D exploration survey may cover many square miles and consist of many shots and receivers deployed in a surficial array. The amount of data produced is staggering and its processing in order to unveil the internal structure of the earth is one of todays grand challenge computational problems.

Ray tracing is used to simulate some aspects of this process. For instance, it can be used for survey planning, by constructing the best model of a geologically complex target and running what/if experiments, to indicate what deployment of charges and sensors will best illuminate the target area.

Once the data has been collected, ray tracing can be used to map from time to depth interpreted events corresponding to strong coherent reflections from targets of interest. A more sophisticated automatic model correction can be also carried out with ray tracing by using full nonlinear travel time inversion. This procedure can be usefully coupled to more conventional processing like time or depth migration that requires good velocity models to succeed. Some migration methods also require extensive travel time tables that again can be generated by efficient ray tracing methods. Given a good velocity model, ray tracing can be employed to identify particular events, either in data or in more complete finite element calculations [11].

In earthquake seismology the basic problem is similar but usually the scale is much larger, the data is less regular and Nature made, and the some of the questions and emphasis are different [9, 14].

In nondestructive evaluation, ultrasound probes are used to find defects in mechanical parts. The probes are piezoelectric transceivers and the scale is in the order of meters rather than kilometers. In the applications we have been involved, both the media and the geometry of the parts is complex.

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