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Numerical Methods in Seismology

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A survey is given of the numerical methods used for computing synthetic seismograms. In particular, the properties of finite differences, finite elements, integral transforms, and ray tracing are described. Each of these methods is capable of giving good results for its own range of frequencies and wave numbers. Thus, for complete seismograms, one should be prepared to use all of the available tools.

1. INTRODUCTION

This report presents a survey of computational techniques used in solving the elastodynamics equations in seismology. At the present time there exists no one method capable of computing complete synthetic seismograms accurately and efficiently for the elastic wave equation with a source having both high and low frequency behavior. We discuss here many methods, each of which is applicable to a particular range of parameters.

We discuss the advantages and disadvantages of the most common methods used in computational seismology: finite differences and finite elements, integral transforms, and ray tracing. Each of these methods has a corresponding set of problems for which it is the best one to use. It is also clear that someone who knows both numerical analysis and geophysics could easily make substantial increases in the computational efficiency of each of these methods. When we are interested in high frequency or first motion response, we might well use asymptotic ray theory for an inhomogeneous medium and the generalized ray theory for a vertically stratified medium. For the long time and the low-frequence response, modal expansion of the solution is appropriate in a stratified medium. When the medium is laterally heterogeneous, a discrete coordinate method (finite difference or finite elements) is useful.

We list some limitations of the methods. It is numerically inefficient to apply a modal expansion method or discrete coordinate methods (finite differences or finite elements) to compute the high-frequency response. The reason is that the resolution of a rapid variation would require the use of higher modes or the use of small mesh widths. The application of an asymptotic ray method to smoothly varying phenomena

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encounters multiple turning of the rays and, therefore, caustic surfaces, at which point the method breaks down. The limitation on the generalized-ray method is that in a many-layered model there are far too many rays for efficient computation.

Integral transform methods also have limitations. They can provide accurate results over certain regions of the parameter space but not all regions. An integral transform method gives an integral representation of the solution. An accurate approximation can be efficiently obtained by using asymptotic expansion of integrals for the far field and long-time solutions. For the short time or the near-field behavior, other approximate methods must be used. In these ranges of parameters, the solutions have simple analytic representations. The midfrequency or the intermediate regions are inaccessible to approximate analytic treatment, but they are favorable to direct numerical solution.

Our principal conclusion is that there exists no single method which can compute with efficiency and with uniform accuracy the response of an inhomogeneous elastic medium to an arbitrary source with a spectrum of frequencies. An efficient and accurate general software package must be a hybrid of many computational procedures. Such a package is yet to be developed.

We begin with a discussion of finite differences and finite elements. We treat them together because they are very similar, in spite of the fact that small differences are very important to the true believers. In fact, if either camp were to adopt the best features of the other camp, the methods would be greatly improved. The circumstances for which these methods are most suitable are short time and short-range computation of smooth waves in an arbitrary medium.

We then discuss integral transform methods. They are restricted to special geometry, such as horizontal stratification. From a numerical point of view these methods require the numerical evaluation of inverse transforms and the solution of a two-point boundary value problem for a system of ordinary differential equations. For a stack of homogeneous layers the two-point boundary value problem is equivalent to a matrix problem. We comment on numerical difficulties and on the geophysical interpretation of numerical methods. For example, poles correspond to modes, and iterative schemes for the matrix correspond to generalized rays.

Finally, we examine ray tracing methods. They may be used in arbitrary geometries but they are a high-frequency asymptotic approximation. It is easy to track rays without regard to the final destination. If we track ray tubes, it is also quite easy to obtain ray amplitudes, again, letting the rays go where they will. If, on the other hand, we want a ray which reaches a particular receiver, we must solve a two-point boundary value problem. This is more difficult and we point out that the effort involved in hitting a specified receiver gives the ray amplitude with little extra computation.

2. Discrete Coordinate Methods

In this section we first discuss finite-difference methods, with emphasis on numerically-induced dispersion and numerical boundary conditions. These considerations apply to finite-element methods as well, but finite-element methods have further special characteristics, which are discussed in Section 2.5.

The main advantage of finite-difference methods is that they may be used to track seismic waves in structures of arbitrary geometry. In particular, in contrast to integral-transform methods, they have no restriction to stratified layers. It is true that ray tracing methods also are valid in structures of arbitrary geometry, but they represent a high-frequency asymptotic approximation. The main disadvantage of finite-difference methods is that they necessarily introduce some dispersion, and they frequently also have some dissipation. Let us point out that one manifestation of cumulative dispersion is dissipation.

Another peculiarity of finite-difference schemes is that they sometimes require more boundary conditions than the corresponding physical problem. Ordinarily, this causes no difficulty because the extra boundary conditions may be obtained by extrapolation. The main requirement is to be aware of the problem. We shall discuss the need for extra numerical boundary conditions and make comments on various extrapolation methods. There is an extensive theory on the interaction between extrapolation at the boundaries, numerical dispersion, and stability.

2.1. *Numerically-Induced Dispersion*

In a linear elastic solid, waves propagate at precisely two speeds, the speed of shear waves and the speed of compression waves. In a difference scheme, however, there is a continuum of wave speeds so that waves in a finite-difference grid act like waves in a crystal lattice. The characteristic of dispersive waves is that individual wavelets move at one speed (the phase velocity), while wave packets move at another speed (the group velocity). Because the energy moves at the group velocity, it is the group velocity which is physically important (Brillouin [12]). In most discussions of numerically-induced dispersion in numerical analysis journals it is only the phase velocity which is mentioned. The most important exception to this misdirected emphasis is the very nice review paper (Trefethen [89]).

As an example which shows numerically induced dispersion, let us consider a discretization of the acoustic wave equation $u_{tt} = c^2 u_{xx}$ by the method of lines

$$\ddot{u}_k = (c^2/h^2)(u_{k+1} - 2u_k + u_{k-1}). \tag{2.1}$$

Here, for simplicity we have discretized x only, with $x_k = kh$ and $u_k = u(x_k, t)$. Even so, this example has the basic properties of the method of Alterman and Loewenthal [3]. By scaling the time $\tau = ct/h$, equation (2.1) becomes

$$d^2 u_k/d\tau^2 = u_{k+1} - 2u_k + u_{k-1}. \tag{2.2}$$

This form emphasizes the dimensionless parameter $\tau = ct/h$, which measures the number of grid lines the wave has passed.

Equation (2.2) is most easily analyzed in terms of its discrete Fourier transform

$$\tilde{u} = \sum u_k e^{-ik\xi}. \tag{2.3}$$

Thus multiplying (2.2) by $e^{-ik\xi}$ and summing yields

$$\begin{aligned} d^2\tilde{u}/d\tau^2 &= -2(1 - \cos\xi)\,\tilde{u} \\ &= -4\sin^2(\xi/2)\tilde{u}. \end{aligned}$$

The general solution of this equation is

$$\tilde{u} = A(\xi)\exp\{i\tau\, 2\sin(\xi/2)\} + B(\xi)\exp\{-i\tau\, 2\sin(\xi/2)\}.$$

Since the inverse transform of (2.3) is

$$u_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{u}(\xi)\, e^{ik\xi}\, d\xi.$$

With $x_k = kh$ we have

$$\begin{aligned} u_k = &\frac{1}{2\pi}\int_{-\pi}^{\pi} A(\xi)\exp[(ict/h)(2\sin(\xi/2) + \xi x_k/(ct))]\, d\xi \\ &+ \frac{1}{2\pi}\int_{-\pi}^{\pi} B(\xi)\exp[(-ict/h)(2\sin(\xi/2) - \xi x_k/(ct))]\, d\xi. \end{aligned} \tag{2.4}$$

We may analyze the integrals in (2.4) by the method of stationary phase or, equivalently in this case, the saddle-point method. Thus, the phase function for the second integral in (2.4) is

$$\phi(\xi) = 2\sin(\xi/2) - x_k\xi/(ct),$$

and the saddle points or points of stationary phase are the values of ξ_0 at which $\phi'(\xi_0) = 0$. That is, ξ_0 satisfies the equation

$$\cos(\xi_0/2) = x_k/(ct). \tag{2.5}$$

From standard asymptotic analysis (Brillouin [12]) condition (2.5) says that given x and t with $|x|/(ct) < 1$ and for $ct/h \to \infty$, the second integral in (2.4) is asymptotic to

$$\text{const.}(h/t)^{1/2}\,|\phi''(\xi_0)|^{-1/2}\, B(\xi_0)\exp\{-ict\phi(\xi_0)/h\}.$$

This may be viewed as saying that for given speed x_k/t, the wave packet moving at that speed has wave numbers centered about ξ_0 given by (2.5). In other words, the group velocities are $c\cos(\xi_0/2)$. Thus, the group velocities range from $-c$ to c.

From a Taylor expansion of the cosine for wave number ξ_0 near zero, the group velocity is

$$c(1 - \xi_0^2/8 + \cdots)$$

which is close to c. Note that by (2.3) $1/\xi_0$ may be regarded as the number of points per wave length. It is a rule of thumb among computational physicists that in practice one should take $\xi_0 \leqslant 0.1$ (at least 10 points per wave length). In fact, this rule is not rigid. For schemes with higher order of accuracy one may relax it to perhaps $\xi_0 \leqslant 0.15$; see Swartz and Wendroff [85].

Another reason not to hold fast to the $\xi_0 \leqslant 0.1$ rule is that the numerical dispersion is cumulative as t increases, but this effect goes as (ct/h) to a fractional power. This phenomenon is most easily seen in terms of a heuristic analysis via Taylor approximation to the difference scheme (2.1) (Chin and Hedstrom [21]). We may use

$$u_{k\pm 1} = u \pm hu_x + (h^2/2)\, u_{xx} \pm (h^3/6)\, u_{xxx} + (h^4/24)\, u_{xxxx} + \cdots,$$

to see that smooth solutions to (2.1) actually approximate the differential equation

$$u_{tt} = c^2(u_{xx} + h^2/12 u_{xxxx}). \tag{2.6}$$

Here, we have truncated the infinite series at the first correction term.

The Fourier transform

$$\hat{u}(\xi, t) = \int_{-\infty}^{\infty} u(x, t)\, e^{-i\xi x}\, dx$$

of the solution u of (2.6) is given by

$$\hat{u}(\xi, t) = A(\xi) \exp\{ict\xi(1 + h^2\xi^2/12)^{1/2}\} + B(\xi) \exp\{-ict\xi(1 + h^2\xi^2/12)^{1/2}\}.$$

for some functions A and B. To within the accuracy of the expansion (2.6) (for $h\xi$ small) this is

$$\hat{u}(\xi, t) \approx A(\xi) \exp\{ict\xi(1 + h^2\xi^2/24)\} + B(\xi) \exp\{-ict\xi(1 + h^2\xi^2/24)\}. \tag{2.7}$$

The inverse Fourier transform of (2.7) is a pair of Airy integrals. In fact, with a change of variable

$$\xi = (cth^2/8)^{-1/3}\, \eta;$$

the inverse transform of the second term on the right-hand side of (27) is the Airy integral

$$(cth^2/8)^{-1/3} \int_{-\infty}^{\infty} B(\xi) \exp\{i(\omega\eta - \eta^3/3)\}\, d\eta$$

with

$$\omega = \left(\frac{x-ct}{h}\right)\left(\frac{8h}{ct}\right)^{1/3}.$$

We see that the dispersion increases with t as $t^{1/3}$. We also see that the dispersion depends on two dimensionless parameters, the distance from the wave front $(x-ct)/h$, and the number of mesh points that the wave has traversed ct/h.

For schemes with different order of accuracy the fractional exponent is different, but the effect is the same (Chin and Hedstrom [21]). The point is that as we track a wave for longer and longer times, we need to increase the number of points per wavelength.

We have discussed dispersion for a method of lines with discretization of x only. The analysis of a full difference scheme is similar but the algebra is more messy. The above considerations apply equally well to the elastic wave equations. The main difference is that for commonly used schemes the shear waves undergo more numerical dispersion than longitudinal waves.

Finally, we would like to warn the reader that the use of elaborate methods may lead to the introduction of parasitic waves. Some examples are given by Okrouhlik [67], Okrouhlik and Brepta [68], and Hedstrom [42].

2.2. *Extra Boundary Conditions*

Boundary conditions needed to solve the partial differential equation must also be used in the difference scheme. Some difference schemes, though, require extra boundary conditions. Let us illustrate with an example of a difference scheme needing more boundary conditions than the corresponding partial differential equation. The wave equation may be written as a first-order system of equations

$$u_t = v_x, \qquad v_t = c^2 u_x. \tag{2.9}$$

In fact, (2.9) is equivalent to $\phi_{tt} = c^2\phi_{xx}$ if $u = \phi_x$ and $v = \phi_t$.

In order to keep things simple, we discretize in x only,

$$\begin{aligned} \dot{u}_k &= (v_{k+1} - v_{k-1})/(2h), \\ \dot{v}_k &= c^2(u_{k+1} - u_{k-1})/(2h). \end{aligned} \tag{2.10}$$

If the differential equation (2.9) is defined on the half line $x > 0$, then because one wave enters from the boundary $x = 0$, we need one boundary condition, say, $u(0, t) = f(t)$. For the difference scheme (2.10), however, we must have a way to specify $v_0(t)$ in addition to the physical boundary condition $u_0(t) = f(t)$. An extensive theory has been developed dealing with ways to choose $v_0(t)$ in a consistent and stable manner, and the basic paper in the theory is Gustafsson, Kreiss, and Sundström [38]. Trefethen's explanation [89, 90] in terms of group velocity is much easier to understand, however. It turns out that for this particular scheme it is permissible to take simply $v_0(t) = v_1(t)$. From a physical point of view it seems more

satisfying to obtain the extra boundary condition by integrating the outgoing Riemann variable along the characteristic. Thus we might discretize $cu_t + v_t = c(cu_x + v_x)$ by using

$$c\dot{u}_0 + \dot{v}_0 = c(c(u_1 - u_0) + (v_1 - v_0))/h.$$

This boundary condition is also quite satisfactory.

It is worth pointing out that people sometimes use special tricks in order to avoid the need for these extra boundary conditions. We could have written the difference scheme for (2.9) in the form

$$\dot{u}_k = (v_{k+1/2} - v_{k-1/2})/h,$$
$$\dot{v}_{k+1/2} = c^2(u_{k+1} - u_k)/h.$$

For this difference scheme it is very convenient to specify $u(0, t)$, and there is no need to extrapolate v at the boundary. The main drawback with this approach is that it is awkward to specify a boundary condition of the form

$$au + bv = f,$$

because u and v aren't defined at the same grid points. In fact, one very common such boundary condition is the requirement that the incoming characteristic variable be constant or, equivalently, that its time derivative be zero,

$$cu_t - v_t = 0.$$

Physically, this boundary condition says that no waves are reflected from the boundary $x = 0$, so that it gives a transmitting boundary condition. We shall discuss transmitting boundary conditions in more detail later, particularly, extensions to waves in several space dimensions.

The points we wish to make here are that it is often convenient to use a difference scheme which requires numerical boundary conditions in addition to those appropriate for the physical problem, and that it is possible to obtain these extra numerical boundary data by extrapolation of interior values. The basic theory for such extrapolation schemes is the paper of Gustafsson, Kreiss, and Sundström [38], but the clearest exposition of the subject is in Trefethen [89, 90].

2.3. *Numerical Dissipation and Artificial Viscosity*

We make a few comments about numerical dissipation because it is much discussed in the numerical analysis literature. In fact, dissipation is of minor significance in the computation of smooth waves in linear elasticity. In nonlinear waves though, it is so important that it is sometimes added intentionally in the form of an artificial viscosity (Richtmyer and Morton [78]). Thus, in computational seismology the use of artificial viscosity would ordinarily be confined to the computation of large displacements near a source. We mention that for linear wave

propagation numerical dissipation is most troublesome when the spacial mesh is too coarse to resolve the waves (Chin and Hedstrom [21]), but it is hard to see much use in seismology for computations under such conditions.

There is one situation in linear elasticity in which it is advantageous to add a small amount of high-order artificial viscosity, and that is when extrapolation is used to generate boundary conditions required by the difference scheme. It is shown by Trefethen [90] that this extrapolation can cause inaccuracy and even instability if numerical dispersion permits waves to go in the wrong direction and if the extrapolation boundary condition excites one of these wrong-way waves. The advantage of an artificial viscosity is that it dissipates the wrong-way waves which are highly oscillatory in x. (Note though, that we still have to watch out for the occasional wrong-way wave which is smooth in x but highly oscillatory in t (Trefethen [89, 90]). The easiest way to obtain an artificial viscosity appropriate for damping wrong-way waves is exemplified by adding dissipation to (2.9) as in

$$u_t = v_x + a(-1)^{n-1} h^{2n-1} \partial^{2n} u/\partial x^{2n},$$
$$v_t = c^2 u_x + b(-1)^{n-1} h^{2n-1} \partial^{2n} v/\partial x^{2n}.$$

The choice of a and b is best made by doing numerical experiments, because it depends on the difference scheme, the number of grid points per wave length, and the distance over which the wave is to propagated. The factor h^{2n-1} makes the equations scale properly. For linear elasticity we would recommend $n = 2$, and for nonlinear problems with shocks it is necessary to use $n = 1$.

Finally, let us remark that the discussion on numerical dissipation up to this point has been based on the assumption that the dissipation arises from the addition of an artificial viscosity to a nondissipative difference scheme. That approach has the advantage that the user may control the amount of dissipation through the choice of the coefficient of viscosity. There do exist difference schemes which are inherently dissipative, such as upstream differences and the Lax–Wendroff scheme. The easiest way to identify whether a scheme is dissipative and to determine the order and coefficient of the principal dissipative term is to obtain its modified equation (Warning and Hyett [94]) as we did to get (2.6). We shall not pursue this point further, because the difference schemes commonly used for computational seismology are not inherently dissipative.

2.4. *Transmitting Boundary Conditions*

In computational seismology we usually want to compute over a region with artificial boundaries, simply to keep the computational problem to a reasonable size. Thus, we want to impose boundary conditions which let waves pass out without reflection. In one space dimension this is easily accomplished, as mentioned earlier, by keeping the incoming characteristic variables constant in time. In several dimensions, though, this is harder to accomplish because waves come in over the light cone, and we can't handle all incoming directions at once. Engquist and Majda [34] introduced an approximate method for suppressing reflected waves over a

specified range of angles. They worked out these boundary conditions for elasticity in their paper (Engquist and Majda [35]). Further expansion in this direction may be found in Clayton and Engquist [26a]. In a typical application on a rectangular domain they use boundary conditions along a side tuned to transmit waves coming in at near normal incidence. At a corner they make the boundary transmit waves coming near 45° to an edge. Their papers contain computational examples showing the amount of reflection for waves meeting the boundary at angles different from ideal.

Engquist and Majda remark that one could tune the boundary conditions so that all spherical waves emitted from a specific point source are transmitted without reflection. Other waves would be reflected to some degree. They do not work out the details, but this could easily be done using their method. It is clear that for some seismological applications this approximation is more appropriate than the assumption of near-normal incidence.

2.5. *Finite-Element Methods*

The comments we have made on finite-difference methods apply also to finite-elements methods. In fact, it is best to regard finite-element methods as a particular class of generalized finite-difference methods (Swartz and Wendroff [84]). Finite-element methods are usually not dissipative (unless artificial viscosity is added deliberately), so that they exhibit numerical dispersion with a wide range of group velocities (Chin, Hedstrom, and Karlsson [22]). The equations of linear elasticity may be written either as a system of second-order equations or as a system of first-order equations. When the finite-element method is used on the first-order representation, it happens (just as in the finite-difference case) that we need to specify extra numerical boundary conditions beyond those determined by the physics. Trefenthen's analysis of this problem for difference schemes applies just as well to finite-element methods (Trefethen [89, 90]). An analysis of this question for finite element methods was given by Strikwerda [83], but Strikwerda's analysis should be combined with Trefethen's insight for an understanding of the mechanism operating here.

Let us use the acoustic wave equation in one space dimension to explain why the finite element method might need extra boundary conditions. Most commonly, the finite element method uses piecewise-linear basis functions ϕ_k as in Fig. 1. We approximate u in

$$u_{tt} = c^2 u_{xx} \tag{2.11}$$

by finite elements

$$u = \sum a_k(t)\, \phi_k(x), \tag{2.12}$$

multiply by ϕ_j, and integrate over x. Note that substitution of (2.12) into (2.11) is only formal because ϕ_k'' doesn't exist in the usual sense. This difficulty is resolved by a formal integration by parts

$$\int c^2 \phi_k'' \phi_j \, dx = -\int \phi_k' (c^2 \phi_j)' \, dx,$$

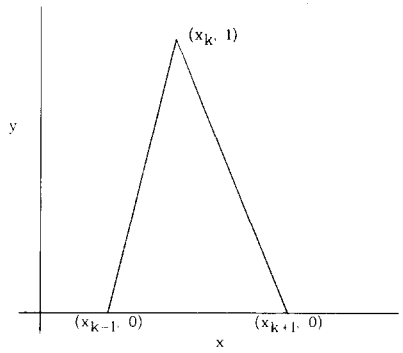

FIG. 1. Finite-element basis function φ_k.

and this latter integral is well defined if c^2 is differentiable. Thus, the finite-element method for (2.11) is

$$\sum_k \frac{d^2 a_k}{dt^2} \int \phi_k \phi_j \, dx = -\sum_k a_k \int \phi_k' (c^2 \phi_j)' \, dx. \tag{2.13}$$

Note that in static problems it is common to derive the finite-element method via a minimum principle. For time-dependent problems we have to use an approach equivalent to that given here.

In order to better display some of the peculiarities of finite-element methods, we calculate the integrals in (2.13) when c is constant and the mesh is uniform $x_{k+1} - x_k = h$,

$$(\ddot{a}_{k-1} + 4\ddot{a}_k + \ddot{a}_{k+1})/6 = c^2 (a_{k+1} - 2a_k + a_{k-1})/h^2. \tag{2.14}$$

For an initial-boundary-value problem on $0 \leqslant k \leqslant K$ for (2.14) we need to specify initial data $a_k(0)$ and $\dot{a}_k(0)$ and boundary data $a_0(t)$ and $a_K(t)$. Since $u(x_k, t) = a_k(t)$ in (2.12), this is just the same data as are suitable for (2.11).

For the sake of comparison let us present the finite-element method for the first-order version (2.9) of the acoustic wave equation. If we replace v by

$$v = \sum b_k(t) \, \phi_k(x)$$

and use (2.12) to represent u in (2.9), multiply by ϕ_j, and integrate, we get the finite-element equation

$$\sum_k \frac{da_k}{dt} \int \phi_k \phi_j \, dx = \sum_k b_k \int \phi_k' \phi_j \, dx,$$

$$\sum_k \frac{db_k}{dt} \int \phi_k \phi_j \, dx = \sum_k a_k \int c^2 \phi_k' \phi_j \, dx.$$

In the particular case when c is constant and the mesh is uniform, this becomes

$$(\dot{a}_{k-1} + 4\dot{a}_k + \dot{a}_{k+1})/6 = (b_{k+1} - b_{k-1})/(2h)$$

$$(\dot{b}_{k-1} + 4\dot{b}_k + \dot{b}_{k+1})/6 = c^2(a_{k+1} - a_{k-1})/(2h).$$

As we saw for (2.10), we find that at a boundary, say $k = 0$, for (2.15) we must specify both $u(0, t) = a_0$ and $v(0, t) = b_0$, which would overdetermine (2.9). Thus, one of these boundary values has to be extrapolated from the interior.

For historical reasons finite-element programs tend to have more flexible grid structure than finite-difference methods. This is because the first use of finite-element methods was in the modeling of structures, and a lot of effort was devoted to making the grids fit the structures. Certainly, finite-difference grids can be just as flexible, but so far, flexible finite-difference grids are mainly found in aerodynamical computations (Thompson *et al.* [88]). The need for flexible grids arises, for example, when we want to compute seismic waves in a structure made up of two materials separated by a dome-shaped boundary. Experimental computations show that in this case we must ue a grid adapted to the boundary surface in order to avoid numerically induced scattering from the interface.

We must comment on some practical special aspects of finite-element methods. A finite-element method converts a partial differential equation into a large system of ordinary differential equations, one equation for each grid point. If an explicit method is used to solve this system of ordinary differential equations, then the time step must be significantly smaller than would be needed for a standard finite-difference method (Chin, Hedstrom, and Karlsson [22]). This turns out to be a minor inconvenience, though, because finite-element methods naturally call for implicit methods. This is because the system of ordinary differential equations to be solved is always of the form seen in (2.14) and (2.15)

$$A\dot{u} = f(u).$$

Here, A is a nondiagonal matrix called the mass matrix. Thus, if u^n denotes an approximation to $u(x, t_n)$ then a typical difference scheme in time will be something like

$$A(u^{n+1} - u^n)/\Delta t = \theta f(u^{n+1}) + (1 - \theta) f(u^n), \tag{2.16}$$

where θ is a parameter. We see that even for an explicit scheme $\theta = 0$, we have to solve a matrix equation $Au^{n+1} = B$ at every time step. It is true that some two and three-dimensional finite element codes simply replace A by a diagonal matrix. This is called "mass lumping." In mass lumping, off-diagonal terms in the mass matrix are moved to the diagonal so that the lumped version of (2.14) is

$$\ddot{a}_k = c^2(a_{k+1} - 2a_k + a_{k-1})/h^2,$$

which is just the common finite-difference scheme (2.1). Similarly, mass lumping of (2.15) produces (2.10). The effect of mass lumping is to reduce accuracy (Cullen [31]) in exchange for a reduction in computer time. It turns out to be about an even trade provided that the matrix problems are solved by an iterative method.

As we have seen, the finite-element method naturally leads to the necessity to solve a matrix equation at each time step. There are, of course, many ways to solve matrix equations. The finite-element is such that in each row of A only the diagonal entry and a few of the off-diagonal entries are nonzero. In fact, for 1-dimensional problems the nonzero entries all lie in a band about the main diagonal, and the same is true of the entries coming from $\theta f(u^{n+1})$. Thus, Gaussian elimination is fast and cheap for the 1-dimensional finite-element time-integration matrix problems.

In two space dimensions it has been standard practice in finite-element codes to still use Gaussian elimination, even though the nonzero entries of A are more widely scattered. Finite-element practitioners have devoted much effort to developing automatic algorithms for reordering the unknowns so as to minimize the storage and work required in the Gaussian elimination. On sequential computers this approach is adequate for small problems, but iterative schemes are much easier to vectorize and they require far less memory capacity. For three-dimensional problems it is imperative to use iterative methods for solving the matrix problems, even on sequential computers. It should be remembered that in these problems the iterative scheme need not be carried out to complete convergence and, in fact, it is foolish to do so because the difference scheme itself has some inaccuracy (Cullen [31]). For a vector computer, the advantage of iterative schemes over Gaussian elimination is even greater.

We may say that the finite-element method is a reasonable thing to use in computational seismology provided that we do not use mass lumping, that we use an implicit scheme to do the integration in time, and that we use an iterative scheme to solve the resulting matrix problem. The main advantage of the finite-element method is that it usually has the capacity to generate a grid adapted to the geometry. It may be noted that the finite-element method used by Lysmer and Drake [61] uses mass lumping and an explicit time-integration scheme.

2.6. *Spectral Methods*

As we have noted, the main disadvantage of finite difference and finite-element methods for computational seismology is their numerically induced dispersion. One way to avoid this problem is to use the spectral method, in which a spatial derivative is computed by taking a Fourier transform, multiplying by $i\xi$, and Fourier transforming back. Because fast Fourier transform routines exist, this method is not as expensive as it might seem at first glance. Furthermore, on a rectangular domain the process is easily vectorized. For meteorological computations the spectral method is quite popular and it is competitive with finite-difference methods (Cullen *et al.* [30]). It should be remembered that on the globe boundary conditions are no problem. In seismology, however, boundary conditions are typically incompatible with spectral methods.

2.7. *Current Research in Numerical Methods*

For finite-difference methods the primary need is the ability to easily generate grids compatible with the geometry, as is currently done with finite elements. Certainly, one could pull the grid-generation portion out of a finite-element code and use it for finite differences. (In effect, this is what mass lumping in a finite-element code boils down to.) Some adaptive grid codes do exist (Thompson *et al.* [88]), but they are not yet used in seismology.

In finite-element codes we have to replace Gaussian elimination with an iterative method, as is standard in finite-difference methods (Hageman and Young [39]). It is not clear at this point what are the best iterative schemes for these problems. The theory of iterative schemes is well developed for positive-definite symmetric matrices. If the equations of linear elasticity are written as a second-order system, the resulting matrix problem for an implicit-time scheme for the finite-element system is symmetric and positive definite, and we may use any standard iterative scheme. If the elastic equations are written as a first-order system, though, the corresponding matrix for a time-implicit scheme for the finite-element method has a matrix which is positive definite but not symmetric. The mass matrix A in (2.16) is symmetric and positive definite. The term $\theta f(u^{n+1})$ is symmetric and negative definite for the second-order equation (2.14), but for the first-order system (2.15) it is antisymmetric. Thus, from the point of view of the matrix problem we ought to use the second-order form of the partial differential equations. From the point of view of accuracy, though, the first-order representation is better, because the finite-element method is more accurate for first-order equations than for second-order equations (Thomée and Wendroff [87]). This is a question which can only be settled by experience.

For the longer term for both finite difference and finite-element methods, we should keep in mind the ongoing developments of adaptive-grid methods which automatically adjust the grid to put a fine mesh wherever resolution is needed. For a survey of current research in this direction see the review article (Hedstrom and Rodrigue [43]). For seismological computations it seems likely that some form of wave tracking is necessary.

3. Integral Transform Methods

Integral transform methods can provide an accurate and efficient technique of obtaining the solution to the equations of elastodynamics in certain regions of the parameter space. Any particular approximation method for the integral will, however, be very inefficient for some values of the parameters. For example, efficient and accurate solutions may be obtained using asymptotic expansions of integrals for the far field and long-time solutions. On the other hand, the modal expansion is appropriate for the long time low-frequency response in a stratified medium. In this range of parameters, the solutions have simple representations. The midfrequency or intermediate regions of the parameter space are inaccessible to approximate analytic treatment but are favorable to direct numerical solutions.

Historically, the integral transform methods have been used because they give integral representations of the solution that can be exploited using asymptotic expansions to extract details of the physical behavior of waves in stratified media. A familiar form of the integral transform representation is given by Woodhouse [97],

$$\mathbf{u}(r, \theta, z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \exp(i\omega t) \int_0^{\infty} \sum_m (\tilde{U}\mathbf{R}_k^m + \tilde{V}\mathbf{S}_k^m + \tilde{W}\mathbf{T}_k^m)\, k\, dk, \tag{3.1}$$

$$\boldsymbol{\sigma}_z(r, \theta, z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \exp(i\omega t) \int_0^{\infty} \sum_m (\tilde{P}\mathbf{R}_k^m + \tilde{S}\mathbf{S}_k^m + \tilde{T}\mathbf{T}_k^m)\, k\, dk, \tag{3.2}$$

where

$$\mathbf{R}_k^m = \mathbf{e}_z J_m(kr) \exp(im\theta),$$

$$\mathbf{S}_k^m = \frac{1}{k} \nabla_1 [J_m(kr) \exp(im\theta)],$$

$$\mathbf{T}_k^m = -\frac{1}{k} \mathbf{e}_z \times \nabla_1 [J_m(kr) \exp(im\theta)],$$

and

$$\nabla_1 = \mathbf{e}_r \frac{\partial}{\partial r} + \mathbf{e}_\theta \left(\frac{1}{r}\right) \frac{\partial}{\partial \theta}.$$

Clearly, the representations (3.1) and (3.2) exhibit some of the inherent difficulties associated with their evaluation over the complete parameter space. The Bessel function is a highly oscillatory function for large arguments, and it is well known that the evaluation of oscillatory integrals presents difficulties. Further, the elastic wave response is causal, giving rise to difficulties in numerically evaluating the inverse Hankel and Fourier transforms. For example, the numerical evaluation of the integral must be done over a finite interval (k_1, k_2). If the interval is too small, not only do we leave out significant physical arrivals, but we also produce aliasing, leading to noncausal arrivals at the beginning of the seismogram that many distort the signal of interest. The same phenomenon occurs in FFT analysis if the signal being modeled is larger than the allotted time window. A third problem that is not explicitly exhibited in Eqs. (3.1) and (3.2) is the behavior of the terms in the integrand multiplying the Bessel function, i.e., the behavior of $\tilde{U}$, $\tilde{V}$, $\tilde{W}$, $\tilde{P}$, $\tilde{S}$, and $\tilde{T}$. These functions contain singularities on the real (wave number) k axis. Obviously, a straightforward quadrature along the real k axis can be inaccurate. For a discussion of the difficulties involved in the numerical quadrature see, for example, the papers of Chapman [20].

elastodynamics progresses in two stages. We construct the response functions $(\tilde{U}, \tilde{V}, \tilde{W})$ by solving a two-point boundary value problem, and then we generate the displacements by integrating this response over wave number and frequency.

In this section we discuss these two problems separately to elucidate where the method gives accurate solutions and why it is inefficient in other regions of the parameter space. From this discussion, it will become apparent that a certain number of points per wave length is necessary to adequately represent the wave propagating in a medium, regardless of the technique used to generate the response. In the finite element and finite-difference methods, this fact is well recognized. Integral transform methods are no exception. The need for resolution manifests itself through the step size used to sample the integrands in the systems (3.1) and (3.2) over different regions of the parameter space.

3.1. *Boundary Value Problem*

Using the eigenfunction expansions given by Eqs. (3.1) and (3.2), we obtain from the equations of elastodynamics in a cylindrical coordinate system the system of ordinary differential equations

$$\frac{d}{dz}\begin{bmatrix}\tilde{U}\\ \tilde{V}\\ \tilde{P}\\ \tilde{S}\end{bmatrix}=\begin{bmatrix}0 & k\left(1-2\dfrac{\mu}{\lambda+2\mu}\right) & \dfrac{1}{\lambda+2\mu} & 0\\ -k & 0 & 0 & \dfrac{1}{\mu}\\ -\rho\omega^2 & 0 & 0 & k\\ 0 & -\rho\omega^2+4k^2\mu\left(1-\dfrac{2\mu}{\lambda+2\mu}\right) & -k\left(1-\dfrac{2\mu}{\lambda+2\mu}\right) & 0\end{bmatrix}\begin{bmatrix}\tilde{U}\\ \tilde{V}\\ \tilde{P}\\ \tilde{S}\end{bmatrix}$$

or

$$\frac{d\mathbf{B}}{dz}=\mathbf{AB}+\mathbf{S} \tag{3.3}$$

for the P–SV system. A similar but a smaller system exists for the SH case. The boundary conditions are: (1) no incoming wave from infinity, and (2) zero traction vector $(\tilde{P}, \tilde{S})$ at the free surface. The above system constitutes a two-point boundary value problem. The boundary value problem for Eq. (3.3) in a stratified medium may be solved directly using a number of well-known numerical methods (Keller [51, 52]). It may be solved also by approximating the coefficients of the differential equation so that the resulting boundary value problem is easily solved (Preuss [77]).

The constant layer approximation is an example of approximating the coefficients of the differential equation. Here, the continuously stratified medium is approximated by a piece-wise constant function. The resulting equation has constant coefficients in each subinterval. Preuss [77] gives a precise error estimate for this method.

Let us change coordinates within a layer,

$$\mathbf{B}^i=\mathbf{D}^i\mathbf{V}^i, \qquad i=1, 2,..., N.$$

Substituting into (3.3) we get

$$\frac{d\mathbf{V}^i}{dz} = \mathbf{\Lambda}^i \mathbf{V}^i + \mathbf{S}^i, \tag{3.4}$$

and if

$$\mathbf{D} = \begin{bmatrix} v_\alpha & k & v_\alpha & k \\ -\kappa & -v_\beta & k & v_\beta \\ -\mu(2k^2 - \omega^2/\beta^2) & -2\mu k v_\beta & \mu(2k^2 - \omega^2/\beta^2) & 2\mu k v_\beta \\ 2\mu k v_\alpha & \mu(2k^2 - \omega^2/\beta^2) & 2\mu k v_\alpha & \mu(2k^2 - \omega^2/\beta^2) \end{bmatrix}$$

then $\mathbf{\Lambda}$ is the diagonal matrix

$$\mathbf{\Lambda} = \operatorname{diag}(-v_\alpha, -v_\beta, v_\alpha, v_\beta)$$

with

$$v_\alpha = (k^2 - \omega^2/\alpha^2)^{1/2} \qquad \text{and} \qquad v_\beta = (k^2 + \omega^2/\beta^2)^{1/2}.$$

We note that the matrices $\mathbf{D}$ and $\mathbf{\Lambda}$ contain radicals v_α and v_β. Branch points exist at the four points $k = \pm\omega/\alpha_{N+1}, \pm\omega/\beta_{N+1}$, at which $v_\alpha = 0$ or $v_\beta = 0$. Here, α_{N+1} and β_{N+1} are the P and S wave speeds in the underlying half space. When the choice of branches of v_α and v_β is unrestricted, the integrands in Eqs. (3.1) and (3.2) are four-valued functions of k and must be represented by a four-leaved Riemann surface. We choose branches such that $\operatorname{Im} v_\alpha \geqslant 0$ and $\operatorname{Im} v_\beta \geqslant 0$ to restrict integration to the top leaf. With this restriction, the branches of v_α and v_β are

$$\begin{aligned} v_\alpha &= \sqrt{k^2 - \omega^2/\alpha^2}, & k > |\omega|/\alpha, \\ &= i\sqrt{\omega^2/\alpha^2 - k^2}, & k < |\omega|/\alpha, \\ v_\beta &= \sqrt{k^2 - \omega^2/\beta^2}, & k > |\omega|/\beta, \\ &= i\sqrt{\omega^2/\beta^2 - k^2}, & k < |\omega|/\beta, \end{aligned}$$

$$\alpha = \sqrt{(\lambda + 2\mu)/\rho},$$

and

$$\beta = \sqrt{\mu/\rho}.$$

Thus, in the propagator formulation outside the source layer, the solution of (3.4) may be expressed

$$\mathbf{v}^i(z) = \exp[\mathbf{\Lambda}(z - z_{i-1})]\, \mathbf{V}^i(z_{i-1}^+), \qquad z_{i-1} < z < z_i. \tag{3.5a}$$

The solution

$$\mathbf{B}^i(z) = \mathbf{D}^i \mathbf{V}^i(z) \tag{3.5b}$$

contains growing and decaying exponentials for evanescent waves. Using the continuity of the displacement-traction vector at the layer interfaces, the solution at any level z_i may be obtained from the solution at the adjacent interface z_{i-1} thus giving a matrix two-term recursion relation. This results in the solution being made up of the product of matrices. This is the technique generally used in seismology and represents the Haskell matrix formulation [40]. In the Haskell formulation the response at the interface between the bottom layer and the underlying half space is related to the free-surface response by products of layer matrices. This initial value technique is numerically unstable for high frequencies. The solution is a linear combination of growing and decaying exponentials, giving rise to an ill-conditioned computational procedure for wave amplitudes. The source of this difficulty is a loss of significant digits in forming the linear combination of exponentially large terms of nearly equal magnitude and of opposite signs. The points of this discussion is that the cancellation problem arises naturally in the initial value (or shooting) technique.

From a mathematical point of view, two-term matrix recursion relations tend to have solutions with different growth rates and, unless special measure are taken, numerical methods lose all but the dominant solution (Van der Sluis [92] and Mattheij [63, 64].

In seismology one attempt at avoiding the loss of precision is by the computation of minors of the layer matrices directly, rather than from the elements of the Haskell layer matrices. To see how this works, we note that the columns of the matrix **D** are the eigenvectors of the matrix **A** corresponding to the eigenvalues $\pm\nu_\alpha$ and $\pm\nu_\beta$. Hence the columns of **D** correspond to elementary stress-displacement vectors for up and downgoing P and SV waves. Now, suppose we solve system (3.3) by a shooting technique, beginning at $z = z_{N+1}$ for a fixed value of ω and a trial value of k. Since the system must have only downgoing or decaying waves as $z \to \infty$, the solution for $z > z_{N+1}$ must be a linear combination of the P and SV waves,

$$\mathbf{B}^{(1)} = \begin{bmatrix} \tilde{U}^{(1)} \\ \tilde{V}^{(1)} \\ \tilde{P}^{(1)} \\ \tilde{S}^{(1)} \end{bmatrix} = \begin{bmatrix} \nu_\alpha \\ -\kappa \\ -\mu(2k^2 - \omega^2/\beta^2) \\ 2\mu k \nu_\alpha \end{bmatrix} \exp[-\nu_\alpha(z - z_{N+1})],$$

$$\mathbf{B}^{(2)} = \begin{bmatrix} \tilde{U}^{(2)} \\ \tilde{V}^{(2)} \\ \tilde{P}^{(2)} \\ \tilde{S}^{(2)} \end{bmatrix} = \begin{bmatrix} k \\ -\nu_\beta \\ -2\mu k \nu_\beta \\ \mu(2k^2 - \omega^2/\beta^2) \end{bmatrix} \exp[-\nu_\beta(z - z_{N+1})]$$

corresponding to P and SV waves, respectively. We propagate $\mathbf{B}^{(1)}$ and $\mathbf{B}^{(2)}$ simultaneously from $z = z_{N+1}$ to $z = 0$. The solution to the system is a linear combination of $\mathbf{B}^{(1)}$ and $\mathbf{B}^{(2)}$ for which the stresses must vanish at $z = 0$.

The determinant of the propagated system must vanish, i.e.,

$$D(\omega, k) \equiv \det \begin{bmatrix} \tilde{P}^{(1)} & \tilde{P}^{(2)} \\ \tilde{S}^{(1)} & \tilde{S}^{(2)} \end{bmatrix}_{z=0} = 0.$$

Hence, the solution is obtained by varying k until the determinant $D(\omega, k)$ vanishes. Although the determinant is not large, the individual elements in the determinant are large and many significant figures are lost in calculating $D(\omega, k)$.

Instead of solving for the elements of $\mathbf{B}^{(k)}$, $k = 1, 2$, we may set up equations for the 2×2 minors of $B_i^{(k)}$. We define the 2×2 minors by

$$Y_{ik} = \varepsilon_{\alpha\beta} B_i^{\alpha} B_k^{\beta}, \qquad \alpha, \beta = 1, 2; \quad k = 1, 2, 3, 4,$$

where the alternating tensor $\varepsilon_{\alpha\beta}$ is defined as

$$\boldsymbol{\varepsilon} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

From the above definitions, the determinant $D(\omega, k)$ is given by the value at $z = 0$ of $Y_{34}(\omega, k)$, where the 2×2 minors satisfy the fifth-order system

$$\frac{d}{dz} \begin{bmatrix} Y_{12} \\ Y_{13} \\ Y_{14} \\ Y_{23} \\ Y_{34} \end{bmatrix} =$$

$$\begin{bmatrix} 0 & 0 & \dfrac{1}{\lambda + 2\mu} & \dfrac{1}{\mu} & 0 \\ 0 & 0 & -\dfrac{k\lambda}{\lambda + 2\mu} & -k & 0 \\ -\rho\omega^2 & 2k & 0 & 0 & \dfrac{1}{\mu} \\ \rho\omega^2 - \dfrac{4k^2\mu(\lambda + \mu)}{2\mu} & \dfrac{2k\lambda}{\lambda + 2\mu} & 0 & 0 & \dfrac{1}{\lambda + 2\mu} \\ 0 & 0 & \dfrac{4k^2\mu(\lambda + \mu)}{\lambda + 2\mu} - \rho\omega^2 & \rho\omega^2 & 0 \end{bmatrix} \begin{bmatrix} Y_{12} \\ Y_{13} \\ Y_{14} \\ Y_{23} \\ Y_{34} \end{bmatrix}.$$

Thus the minors are propagated from interface to interface so that disproportionate terms do not appear. This and other modifications to the Haskell formulation, which address the problem of loss of precision with different degrees of success, may be found in the works of Knopoff [58], Dunkin [33], Gilbert and Backus [37], Burridge [13], and Abo-Zena [1]. It is not unreasonable to find that such special tricks do not completely solve the loss-of-precision problem. This is because the minors also satisfy a matrix two-term recursion relation with some growth characteristics. In other words, the minors also have growing and decaying tendencies which must be identified in order to produce a robust computational algorithm.

In the literature on numerical solutions to two-point boundary value problems it is known that multiple shooting techniques can be used to circumvent the difficulties caused by growth of the solutions of the initial value problems to be solved (Keller [51]). For the system (3.3) we prefer the parallel shooting technique in that the difficulty can be eliminated while at the same time it gives a clear physical interpretation of the wave field (Chin, Hedstrom, and Thigpen [23]). In the parallel shooting variant, the boundary value problem is partitioned into subproblems, and the growing solutions in each subinterval are scaled so that the solutions are bounded in magnitude by 1. In other words, we choose a local basis of the linear space of solutions of the homogeneous problem to be uniformly bounded in magnitude by 1. The resultant linear system of equations for the coefficients of the upgoing and downgoing waves is well conditioned.

To get a flavor for this formulation, Eq. (3.5) may be written in the parallel shooting formulation

$$\mathbf{B}^i = \mathbf{D}^i \begin{bmatrix} e^{-v_\alpha^i (z - z_{i-1}^+)} & & & 0 \\ & e^{-v_\beta^i (z - z_{i-1}^+)} & & \\ & & e^{-v_\alpha^i (z_i^- - z)} & \\ 0 & & & e^{-v_\beta^i (z_i^- - z)} \end{bmatrix} \begin{bmatrix} V_\alpha^i(z_{i-1}^+) \\ V_\beta^i(z_{i-1}^+) \\ V_\alpha^i(z_i^-) \\ V_\beta^i(z_i^-) \end{bmatrix}. \tag{3.6}$$

The geometric interpretation is shown in Fig. 2.

In (3.6) the growing exponentials are eliminated. Application of the stress-free boundary conditions at the free surface and the radiation condition at infinity for a

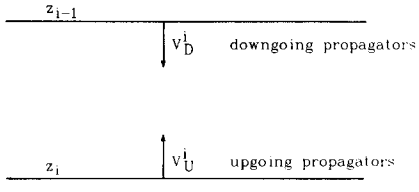

FIG. 2. Upgoing and downgoing propagators.

two-point boundary value problem.

A natural partitioning of the coefficient matrix leads to a block tridiagonal matrix in which off-diagonal blocks contain decaying exponentials in the evansescent regime and the diagonal blocks contain the interface matrices. The vanishing of the determinant of the first matrix on the diagonal gives the Rayleigh wave for the half space, and the vanishing of the determinant of any other diagonal block gives a Stonely wave; see Chin, Hedstrom, and Thigpen [25].

The advantage of the block tridiagonal formulation of the coefficient matrix is that this system is well conditioned. A number of methods can be applied for its solution. For example, the block Gauss–Jacobi iterative method gives a partial generalized ray expansion of the solution (Cisternas, *et al.* [26]). The system may be solved by direct methods such as block LU decomposition or its equivalent, the discrete invariant imbedding method. Discrete invariant imbedding has an immediate physical interpretation in that the solution is written in terms of overall reflection and transmission coefficients. Kennett's [53] technique is just the discrete invariant imbedding algorithm.

For vertically inhomogeneous media, the propagator (3.5) is not particularly useful, as it will be developed in a matrix power series or a matrizant. Treating the differential equations (3.3) directly, Chapman [19] has developed an approximate solution to the vertically inhomogeneous medium by using the Bremmer series (Bremmer [11], Atkinson [7]). The Bremmer series is obtained by changing variables and by using function iteration to solve the resulting ordinary differential equations (3.3) with the WKB solution as the initial iterate. It is clear that the Bremmer series is not uniformly valid in the neighborhood of turning points. The nonuniformity can be circumvented by using a uniformly valid asymptotic expansion (Chapman [18], Wasow [95]) as an initial iterate. Alternatively, we can return to the system (3.3) and solve it by some purely numerical method such as COLSYS (Ascher *et al.* [5]), PASVA3 (Pereyra [74]), or SUPORT (Scott and Watts [82]). The point to remember is that methods differ in efficiency, stability, and ease of application. Any method used to solve the system (3.3) for the response functions should provide a measure of its accuracy and a definition of its region of applicability in the parameter space.

In summary, the construction of the transformed response functions requires that several problems must be addressed in order to obtain an accurate stable solution. A basic difficulty stems from the fact that the earth is not made up of homogeneous layers. An exact analytic solution by the propagator matrix method requires the constant layer approximation. For a vertically inhomogeneous medium, the structure must be replaced by the constant layer approximation for the propagator method to be applicable. High-quality two-point boundary value problem solvers exist which treat vertically stratified media by numerical methods. Finally, one should not restrict oneself to a single technique to solve the problem for the complete parameter space. It is more efficient to use a family of techniques and to select according to model problems whose numerical solution is well understood in the literature.

3.2. *Inverse Transforms*

The form of the integrals to be evaluated in the inverse transformations is [see Eqs. (3.1) and (3.2)]

$$I = \int_{-\infty}^{\infty} \exp(i\omega t)\, d\omega \int_0^{\infty} \frac{g(\omega, k)}{D(\omega, k)} J_n(kr)\, dk.$$

The evaluation of the above integrals is replete with difficulties and has been a major

$g(\omega, k)/D(\omega, k)$ has branch points (points where $v_\alpha = 0$ or $v_\beta = 0$) and poles (zeros of $D(\omega, k)$) on the real k axis, and it is highly oscillatory in some parts of the parameter space considered. Third, the Bessel function is highly oscillatory for large arguments. An additional complication is that aliasing occurs in both k and ω integrations.

In general, one may use one or more of several techniques to evaluate the double integral transforms depending on the frequency and distance range desired. The integrals may be evaluated by asymptotic expansions, by expanding in terms of normal modes, or by direct numerical quadrature. Asymptotic expansions are applicable for large source-receiver distances, high frequencies, and large times after the source has been initiated. Asymptotic expansion techniques use stationary phase or steepest descent methods (Ben-Menahem and Singh [9], Chapman [20], Bleistein and Handelsman [10], Jones [47], and Olver [70]). A solution in terms of normal modes may be obtained for large source-receiver separations and low frequencies. We next examine briefly different techniques used to numerically evaluate the double transform.

3.3. *Shifting off the Axis*

In order to avoid numerical difficulties caused by the poles and branch cuts on the real axis, there are two almost equivalent ways to make the path miss them: by moving the path or by moving the poles and saddle points. If the path is moved into the complex plane, mathematically, the integrals are equal. Phinney [76] did some computations with this method but there is no theory to guide the choice of the distance to move the path off the axis. In fact, the process is equivalent to a filtering and its inverse, in that more information is lost the farther off the axis the path is taken.

The other way that the poles and branch points may be separated from the path is by adding artificial attenuation in analogy with artificial viscosity in finite-difference and finite-element methods. The mechanism used is that of making the modulus complex (Kennett [54]). If the modulus does not satisfy the Kramers–Krönig relation, the solution is no longer causal. In any case the main effect is on the long-time behavior. The main difficulty with this method is that we do not know how much attenuation to introduce; we want to put in enough to reduce the numerical difficulties but not so much that the solution becomes overly smoothed. The paper by O'Neil and Hill [71] has looked at this question a certain amount.

The adherents of these methods feel that they remove the numerical difficulties (Apsel [4], Kind [57], Kennett [56]). It is clear that for some problems this is correct, but we do not know the range of validity.

3.4. *Distortion of the Path*

From a numerical point of view it is better to make a larger distortion of the path than that used by Phinney as discussed in Section 3.3 because this replaces oscillatory exponentials by decaying ones. The best path is one that goes through saddle points and around the branch cuts. We know how to do that for one layer over a half space (Lapwood [59], Newlands [66]). For many layers, however, this is very difficult if not impossible to do because the integrand is the solution of a matrix problem. Herrmann [45] and Wang and Herrmann [93] made a stab at choosing a path, but they still had numerical difficulties.

Let us point out that the location of the branch cuts is at our disposal. Most geophysicists use the cuts introduced by Lapwood [59], even though the integrals along these cuts are highly oscillatory. In electromagnetic theory one takes the cuts straight up or straight down (Jones [47]). We still don't know where to take the cuts in geophysics. Ben-Menahem and Singh [9] take the cuts going straight down.

When we move the path, we must take into account the residues at the poles which the path crosses. These residues represent the trapped modes and the leaky modes, depending on which sheet of the Riemann surface the path is on. In order to find these poles, we must find the zeros of the determinant of the coefficient matrix for the amplitudes of the upgoing and downgoing waves. Schwab and Knopoff [79], Harvey [41], and others claim to have fast methods for finding these zeros.

3.5. *Generalized Rays*

By looking in the proper way at the matrix problem for the amplitudes of the upgoing and downgoing waves, we obtain the generalized ray expansion. From the point of view of numerical analysis we are doing a block Gauss–Jacobi iterative scheme for a matrix problem, and each pair of iterations gives a complete set of multiples. A similar decomposition has been given by Wu and Norwood [98] in terms of three canonical scattering problems. The difficulty with this method is that because of mode conversion it gives far too many rays. Mode conversion further complicates the situation. The traditional geophysical approach (Helmberger [44], Wiggins and Helmberger [96]), is not based on a systematic iterative development of the linear system.

3.6. *Ray–Mode Methods*

The trouble with ray methods is that it takes too many rays to represent the low-frequency aspects of the solution. The trouble with mode expansions is that it takes too many modes to represent the high-frequency aspects of the solution. Consequently, it is natural to use a hybrid ray–mode expansion. For SH waves this has been done by Kamel and Felsen [49].

3.7. *Continuous Gradation*

If the stratified medium is regarded as having continuous variation of material properties instead of being piecewise constant, the Fourier integral transform in time and a vector-harmonic expansion in space produces a two-point boundary value problem for a system of ordinary differential equations. If the coefficients of this differential equation are approximated by piecewise-constant functions, we get the matrix problem considered earlier. Cormier [27] used a piecewise-linear approximation of the coefficients and he was able to obtain a high-frequency asymptotic approximation to the solution via Airy functions. It would be nice to be able to use higher-order approximations to the coefficients, but the resulting two-point boundary value problem is just as difficult to solve as the original one. We can solve this two-point boundary value problem and Ascher and Spudich [6] do just that.

This approach still leaves us with the same double integral to evaluate as we had in the case of a stack of homogeneous layers. We still have modes, and they are more expensive to compute than in the case of homogeneous layers because we need to find eigenvalues of a differential equation. Furthermore, we have no idea where to take the path of integration.

3.8. *Special Methods*

We discuss here some schemes which do not fit into the categories discussed earlier. One is a mixed integral transform and finite difference or finite-element method. The other method uses different approximations in thin layers and thick layers.

Olson, Orcutt, and Frazier [69] use a discrete Hankel transform in the radial direction, leaving a hyperbolic partial differential equation in depth and time. They then solve this partial differential equation using a finite-element method. This approach is very similar to that of Alekseev and Mikhailenko [2], except that this later paper uses finite differences for the partial differential equation. The advantage of this method is that it permits an arbitrary variation of modulus with depth. The main disadvantage is that the schemes for the partial differential equation have inherent numerically induced dispersion, as discussed in Section 2. Another difficulty is that because a discrete transform is used, we get an expansion in terms of the radial eigenfunctions and we have to know the eigenvalues. In these papers the exterior boundary conditions are reflecting, thus limiting the validity of the solution. In summary we may say that this method is good for smooth solutions for times before the first reflection.

Another special method is that of Daley and Hron [32] which used reflectivity in thin layers and rays in thick layers. This avoids the plethora of rays which arises from the multiple reflection in the thin layers. As in the ray–mode method, this is an attempt to provide an approximation which is valid both at high and low frequencies. It seems promising, but perhaps not as good as the ray–mode method.

4. Ray Tracing Methods

In contrast to the discrete coordinate methods (finite difference and finite element) and the integral transform method discussed, we find relatively few discussions of the numerical solution of the ray tracing equations. This section has been purposely expanded to give a thorough discussion of the computational problems in asymptotic ray theory.

The method of solution depends on the intended application. For example, inverting travel time data to study the velocity structure requires ray tracing between specified locations of the source and the receiver. To see how the rays are affected by the velocity structure, we launch a bundle of rays from a given point and trace their path through the medium. This gives a general picture including the location of caustics and shadow zones. Additional insight can be obtained from a ray amplitude computation.

In what follows we examine the effect of these considerations on choosing methods for doing ray tracing.

4.1. *Summary of Asymptotic Ray Theory*

In this section, the asymptotic ray theory or the ray series method is discussed. It is an extension of the Liouville–Green or the WKB method in the asymptotic solution of ordinary differential equations to partial differential equations. In recent years, these techniques for solving problems with disparate scales are called the multiscale expansion methods.

We begin with the postulate that the problem in question has disparate scales. For example, in an inhomogeneous medium the wave speeds may vary more rapidly in some preferred direction giving rise to a layering effect. Let the characteristic length associated with a given variation of the material property or with a distinguished feature of the structure ϕ be denoted by L_ϕ. Then the asymptotic ray theory is developed for phenomena whose characteristic wavelength λ is small compared to the shortest characteristic length of the structure

$$\lambda \ll L = \min_{\phi} L_\phi .$$

Formally, we define the following dimensionless variables denoted by tildes

$$x_i = L\tilde{x}_i, \qquad u_i = u_0 \tilde{u}_i, \qquad t = \frac{L}{c}\tilde{t},$$

$$(\lambda, \rho, \mu) = (\lambda_0 \tilde{\lambda}, \rho_0 \tilde{\rho}, \mu_0 \tilde{\mu}),$$

$$\gamma = \mu_0/\lambda_0,$$

where for a generic variable ϕ on the domain $\Omega \in R^3$

$$\phi_0 = \max_{\Omega} \phi$$

and c is a typical wave propagation speed. Then, the elastodynamic equation becomes

$$\tilde{\rho}\tilde{u}_{i,tt} = \frac{\lambda_0}{\rho_0 c^2}(\tilde{\lambda}+\gamma\tilde{\mu})\,\tilde{u}_{j,ij} + \frac{\mu_0}{\rho_0 c^2}\tilde{\mu}\tilde{u}_{i,jj} + \frac{\lambda_0}{\rho_0 c^2}\tilde{\lambda}_{,i}\tilde{u}_{j,j} + \frac{\mu_0}{\rho_0 c^2}\tilde{\mu}_{,j}[\tilde{u}_{i,j}+\tilde{u}_{j,i}].$$

It is clear from the development that $\lambda_0/\rho_0 c^2$ and $\mu_0/\rho_0 c^2$ are order one quantities.

Consider a development of the solution of the elastodynamics equation in an asymptotic series

$$\tilde{u}_i = \sum_{k=0}^{\infty} U_i^{(k)}(\tilde{\mathbf{x}})\,\varepsilon^k F\left(\frac{1}{\varepsilon}(\tilde{t}-\tau(\tilde{\mathbf{x}}))\right), \tag{4.1}$$

where $\varepsilon = c/\omega L$ and ω is the frequency of interest. Here, c/ω is the wavelength associated with the phenomenon in question, and therefore ε is a ratio of the wavelength to the shortest characteristic length associated with the structure. This is a small number ($\varepsilon \ll 1$) by assumption.

The development of the solution is straightforward and may be found in the literature, for example, Karal and Keller [50], Babich and Alekseev [8], Červený and Ravindra [15], Červený and Hron [14]. A brief summary of the results will be given for the sake of completeness. It should be noted, however, that for the ray expansion to converge it is necessary, by the root test, that

$$\limsup_{k\to\infty} \varepsilon \,\|U_i^{(k)}\|^{1/k} \leqslant 1,$$

where $\|\cdot\|$ is some suitable norm. In the neighborhood of turning points it is well known that the asymptotic ray series diverges. Hence, the ray expansion is not uniformly valid. It must be modified to produce a uniformly valid expansion in the neighborhood of turning points, see Ludwig [60].

In physical variables, the coefficients of the expansion $U_i^{(k)}$ satisfy the following system of equations:

$$N(U_i^{(0)}) = 0, \qquad n = 0, \tag{4.2}$$

$$N(U_i^{(1)}) - M(U_i^{(0)}) = 0, \qquad n = 1, \tag{4.3}$$

$$N_i(U_i^{(n+1)}) - M_i(U_i^{(n)}) + L(U_i^{(n-1)}) = 0, \qquad n \geqslant 2, \quad i = 1, 2, 3, \tag{4.4}$$

where

$$\begin{aligned}
N(V_i) &= -\rho V_i + (\lambda+\mu)\,V_j\tau_{,i}\tau_{,j} + \mu V_i\tau_{,j}\tau_{,j},\\
M(V_i) &= (\lambda+\mu)[V_{j,i}\tau_{,j} + V_{j,j}\tau_{,i} + V_j\tau_{,ji}]\\
&\quad + \mu[2V_{i,j}\tau_{,j} + V_i\tau_{,jj}] + \lambda_{,i}V_{,j}\tau_{,j} + \mu_{,j}V_i\tau_{,j} + \mu_{,j}V_j\tau_{,i},\\
L(V_i) &= (\lambda+\mu)\,V_{j,ij} + \mu V_{i,jj} + \lambda_{,i}V_{j,j} + \mu_{,j}V_{i,j} + \mu_{,j}V_{j,i}.
\end{aligned}$$

Equation (4.2) written in component form is given by

$$\begin{bmatrix} -\rho+(\lambda+\mu)\tau_{,1}^2+\mu\tau_{,k}\tau_{,k} & (\lambda+\mu)\tau_{,1}\tau_{,2} & (\lambda+\mu)\tau_{,1}\tau_{,3} \\ (\lambda+\mu)\tau_{,1}\tau_{,2} & -\rho+(\lambda+\mu)\tau_{,2}^2+\mu\tau_{,k}\tau_{,k} & (\lambda+\mu)\tau_{,2}\tau_{,3} \\ (\lambda+\mu)\tau_{,1}\tau_{,3} & (\lambda+\mu)\tau_{,2}\tau_{,3} & -\rho+(\lambda+\mu)\tau_{,3}^2+\mu\tau_{,k}\tau_{,k} \end{bmatrix} \begin{bmatrix} U_1^{(0)} \\ U_2^{(0)} \\ U_3^{(0)} \end{bmatrix} = \mathbf{0}$$

or

$$\mathbf{A}\mathbf{U}^{(0)} = 0. \tag{4.5}$$

Note that $\mathbf{A}$ is a symmetric matrix. For (4.5) to have a nontrivial solution, the determinant of the coefficient matrix $\mathbf{A}$ must vanish. This yields

$$\left(\tau_{,k}\tau_{,k} - \frac{1}{\alpha^2}\right)\left(\tau_{,k}\tau_{,k} - \frac{1}{\beta^2}\right)^2 = 0.$$

Hence, we have two wave speeds

$$\tau_{,k}\tau_{,k} = \frac{1}{\alpha^2}, \qquad \alpha^2 = (\lambda + 2\mu)/\rho, \tag{4.6}$$

and

$$\tau_{,k}\tau_{,k} = \frac{1}{\beta^2}, \qquad \beta^2 = \mu/\rho. \tag{4.7}$$

Equations (4.6) and (4.7) are known as the eikonal equations. They are first-order hyperbolic equations and may be solved using the method of characteristics. The result is a system of ray tracing equations

$$\frac{dx_i}{d\tau} = v^2 p_i$$

and

$$\frac{dp_i}{d\tau} = -v^{-1}\frac{dv}{dx_i}, \qquad i = 1, 2, 3, \tag{4.8}$$

where $v = \alpha$ or β, and τ is the travel time. Note that

$$\tau_{,k}\tau_{,k} = 1/\beta^2$$

is a double root of the scalar equation $\det(\mathbf{A}) = 0$. Moreover, $U^{(0)}$ still must be determined.

To calculate $\mathbf{U}^{(0)}$, we must solve the next order equation, Eq. (4.3), which is a system of linear equations with a singular coefficient matrix

$$\mathbf{A}\mathbf{U}^{(1)} = \mathbf{M}(\mathbf{U}^{(0)}). \tag{4.9}$$

From the theory of operators in linear spaces (Friedman [36]), the Fredholm alternative holds: the nonhomogeneous equation (4.9) has a solution for a given vector **M** if and only if **M** is orthogonal to every solution of the adjoint homogeneous equation

$$\mathbf{A}^*\mathbf{Z} = 0.$$

Since **A** is real and symmetric, it is self-adjoint. Let a vector in the null space or the kernel of **A** be called a kernel vector. Then, the kernel vector $\mathbf{V}^{(\alpha)}$, corresponding to the root of the secular equation giving the compressional wave, is $(\tau_{\alpha,1}, \tau_{\alpha,2}, \tau_{\alpha,3})$. This is just the normal to the wave front of the compressional wave. It is clearly in the direction of the compressional wave propagation. The two remaining kernel vectors $\mathbf{V}^{(\beta)}$, corresponding to the double root of the secular equation giving the shear waves, lie in the tangent plane to the wave front $\tau_\beta(\mathbf{x})$. This is because

$$(-\rho + \mu\tau_{,k}\tau_{,k})\,\varepsilon_{ilm}\,U_l^{(0)}\tau_{\beta,m} = 0.$$

Here ε_{ilm} is the permutation symbol. Moreover, the vectors $\mathbf{V}_k^{(\beta)}$, $k = 1, 2$, may be taken to be orthogonal.

It can readily be shown that the kernel vectors $\mathbf{V}^{(\alpha)}$ and $\mathbf{V}_k^{(\beta)}$, $k = 1, 2$, are orthogonal along the ray path $\mathbf{x}(\tau)$. This follows from the fact that at any point τ^* along a ray path $\mathbf{x}(\tau)$, $\mathbf{V}^{(\alpha)}(\tau^*)$, $\mathbf{V}_k^{(\beta)}(\tau^*)$, $k = 1, 2$, are the eigenvectors of a real and symmetric acoustic tensor **B** with eigenvalues $\alpha(\tau^*)$ and $\beta(\tau^*)$. The acoustic tensor **B** is given by

$$\begin{bmatrix} (\lambda+\mu)\,n_1^2 + \mu n_k n_k & (\lambda+\mu)\,n_1 n_2 & (\lambda+\mu)\,n_1 n_3 \\ (\lambda+\mu)\,n_1 n_2 & (\lambda+\mu)\,n_2^2 + \mu n_k n_k & (\lambda+\mu)\,n_2 n_3 \\ (\lambda+\mu)\,n_1 n_3 & (\lambda+\mu)\,n_2 n_3 & (\lambda+\mu)\,n_3^2 + \mu n_k n_k \end{bmatrix},$$

where $n_i = \cos\theta_i$ the directional cosines of the propagation vector at $\tau = \tau^*$. The relation between **B** and **A** is $\mathbf{A}(\tau^*) = \mathbf{B}(\tau^*) - \rho(\tau^*)\,v\mathbf{I}$, where v is the eigenvalue. Since **B** is real and symmetric, the eigenvectors associated with different eigenvalues are orthogonal. The triad $\mathbf{V}^{(\alpha)}(\tau^*)$ and $\mathbf{V}_k^{(\beta)}(\tau^*)$, $k = 1, 2$, form a basis at any point τ^* along a ray $\mathbf{x}(\tau)$.

Applying the Fredholm alternative pointwise along a ray $\mathbf{x}(\tau)$, we obtain the following solvability conditions

$$\mathbf{M}(\mathbf{U}^{(0)}) \cdot \hat{\mathbf{V}}^{(\alpha)} = 0$$

and

$$\mathbf{M}(\mathbf{U}^{(0)}) \cdot \hat{\mathbf{V}}_k^{(\beta)} = 0, \qquad k = 1, 2, \tag{4.10}$$

where $\hat{}$ denotes unit vectors. Equations (4.10) are necessary and sufficient for Eq. (4.9) to have a solution. The solution has the representation

$$\mathbf{U}^{(0)} = U_1^{(0)}\hat{\mathbf{V}}^{(\alpha)} + U_2^{(0)}\hat{\mathbf{V}}_1^{(\beta)} + U_3^{(0)}\hat{\mathbf{V}}_2^{(\beta)}.$$

For the higher order equations, equivalent conditions hold,

$$\hat{\mathbf{V}}^{(\alpha)} \cdot \mathbf{N}(\mathbf{U}^{(l-1)}, \mathbf{U}^{(l-2)}) = 0,$$

and (4.11)

$$\hat{\mathbf{V}}_m^{(\beta)} \cdot \mathbf{N}(\mathbf{U}^{(l-1)}, \mathbf{U}^{(l-2)}) = 0, \qquad m = 1, 2, \quad l \geqslant 2,$$

where

$$\mathbf{N}(\mathbf{U}^{(l-1)}, \mathbf{U}^{(l-2)}) = \mathbf{M}(\mathbf{U}^{(l-1)}) - \mathbf{L}(\mathbf{U}^{(l-2)}).$$

This represents a mathematically pleasing derivation of the transport equations (Courant and Hilbert [28]). Note that the ray-centered coordinate system of Červený and Hron [14] follows immediately. As the directions of $\hat{\mathbf{V}}_k^{(\beta)}$, $k = 1, 2$, are at our disposal, they should be chosen to coincide with the polarizations of the shear waves along the ray path.

Upon solving Eqs. (4.10), it is found that the ray amplitude $\mathbf{U}^{(0)}$ for the compressional wave is nonzero only in the direction of wave propagation $\hat{\mathbf{V}}^{(\alpha)}$. This is defined as the principal component of a compressional wave, and the components orthogonal to it are defined as the additional components. On the other hand, the components along the tangent plane of the shear wave front are called the principal components for the shear wave, and the remaining component is called the additional component.The additional component of the zeroth-order shear wave ray amplitude is identically zero. The principal components of the zeroth-order ray amplitudes of both the compressional and shear waves have identical forms,

$$U^{(0)}(\tau) = U^{(0)}(\tau_0) \frac{J(\tau_0)\,\rho(\tau_0)\,v(\tau_0)}{J(\tau)\,\rho(\tau)\,v(\tau)},$$

where $J(\tau)$ and $v(\tau)$ are, respectively, the Jacobian of the transformation from the Cartesian coordinate $\mathbf{x}$ into the ray coordinates (τ, q_1, q_2) and the propagation velocities for compressional and shear waves. The higher-order ray amplitudes are obtained by solving Eq. (4.11). The equations for calculating the ray amplitudes are considerably simplified if a ray-centered coordinate is used with the kernel vectors coinciding with the polarizations of the shear wave.

4.2. *Numerical Methods for Asymptotic Ray Theory*

We now discuss the computational methods for asymptotic ray theory. The method of solution depends on the application. Four possible cases are distinguished:

(1) ray tracing from a specified source location to wherever it wants to go,

(2) ray tracing between specified source and receiver locations,

(3) computing the response from a specified source position along any ray,

(4) computing the response between specified source and receiver locations.

At first glance, case (1) is a subset of case (3). Similarly, case (2) is a subset of case (4). Ordinarily we would do some of these cases in sequence. For a given postulated structure, we first do case (1), sending many rays out from a given source to get a general picture including the locations of caustics and shadow zones. Then we might do case (3) to find ray amplitudes or case (2) to pin down which rays reach a given receiver. Finally, we would do case (4) to obtain the amplitude at a given receiver.

In practice as our discussion will show, tracing rays alone requires different considerations than calculating the response of the medium to a disturbance. The latter situation resuires the solution of the ray tracing equations and the evaluation of the ray amplitudes along a ray. The added task of computing ray amplitudes is extensive and warrants a separate classification. It turns out that the computation involved in tracing a ray from a source to a receiver yields the amplitude with a simple additional calculation.

We will discuss initial and boundary value methods for solving the ray tracing equations. A discussion on ray amplitude will follow. Then ray tracing using the "circular" approximation method is presented.

4.3. *Numerical Solution of the Ray Tracing Equations*

In this section we discuss the numerical solution of the ray tracing equations. The method of solution depends on the application. When it is immaterial where the receiver is located, as in case (1), then the ray tracing problem should be treated as an initial value problem. For applications in which it is imperative that the ray must connect between the source and the receiver, as in Case (2), there are two obvious approaches: (a) formulate the computation as a two-point boundary value problem (Julian and Gubbins [48] and Pereyra, Lee, and Keller [75]) or (b) solve a sequence of initial value problems and then interpolate the results to locate the receiver position, that is, shoot and interpolate.

Two point boundary value methods may be divided into two classes, "shooting" and "nonshooting" (for want of a better term). The shooting method formulates the problem as an initial value problem using the boundary conditions at a given boundary, iteratively varying the remaining parameters so that the boundary conditions at the other boundary point are satisfied. This may be viewed as the finding of a critical set of takeoff angles at the source and total travel time so that a ray will reach the receiver. In fact, the shooting method is a systematic version of method, shoot and interpolate. In the nonshooting or truly two-point boundary value method we begin with an estimate of the solution satisfying all of the boundary conditions and iteratively modify the solution until the differential equations are satisfied.

In the shooting method each iterate satisfies the differential equations but not all of the boundary conditions. In the nonshooting method each iterate satisfies the boundary conditions but not the differential equations. Both methods satisfy the differential equation and the boundary conditions when the iterative scheme has

converged to the true solution. Because of the iterative process, both two-point boundary value methods are computationally expensive.

For a given velocity structure, there may be no ray, one ray, or a number of rays connecting the source to the receiver. This means that the boundary value problem may have multiple solutions. Each solution consists of a takeoff angle and the travel time or total length of a ray. The question of the existence and uniqueness of the solution of the ray tracing boundary value problem has not been solved.

4.4. *Initial Value Problem Formulation*

In this section we give the details of the shooting approach to ray tracing. The ray tracing equations are given by

$$\frac{dx_i}{d\tau} = v^2 p_i, \qquad \frac{dp_i}{d\tau} = -v^{-1}\frac{\partial v}{\partial x_i}, \qquad i = 1, 2, 3. \tag{4.12}$$

This is a system of six nonlinear ordinary differential equations. Here τ is the travel time. This system may be reduced by one by using the eikonal equation

$$p_1^2 + p_2^2 + p_3^2 = \frac{1}{v^2}. \tag{4.13}$$

If the arc length s along the ray path is introduced, i.e.,

$$(ds)^2 = dx_i\, dx_i$$

and

$$\frac{ds}{d\tau} = v,$$

then the ray tracing equations become

$$\frac{dx_i}{ds} = vp_i, \qquad \frac{dp_i}{ds} = -\frac{1}{v^2}\frac{\partial v}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{1}{v}\right), \qquad i = 1, 2, 3. \tag{4.14}$$

Equation (4.14) has been used by Pereyra *et al.* [75].

As an initial value problem, the integration of (4.12) or (4.14) requires six initial conditions

$$x_i(s_0) = x_i^0, \quad i = 1, 2, 3, \qquad \text{and} \qquad p_i(s_0) = p_i^0, \quad i = 1, 2. \tag{4.15}$$

The sixth initial condition is obtained by using the eikonal equation (4.13) evaluated at the initial point s_0 or τ_0. Since the raytracing equations are translationally invariant, we may set $s_0 = \tau_0 = 0$. The initial values x^0 are the coordinates of the

source while p_i^0, $i = 1, 2$, are related to the takeoff angles of the ray. The ray path originating at the source point x_i is, therefore, a function of p_i^0, $i = 1, 2$. The solution of the ray tracing equations is therefore a two-parameter family. The triplet (s, p_1^0, p_2^0) completely characterizes a ray in R^3. This completes the initial value problem formulation if no interfaces are present.

The inclusion of interfaces complicates the situation. When a wave of compression or shear impringes on an interface, mode conversion occurs, namely, two reflected and two refracted waves are generated. A complete discussion of the interface conditions will take us far removed from the central issue of this report. Červený and Ravindra [15] and Červený, Langer, and Pšenčík [16] give clear and lucid discussions. A summary of the results is in order, however.

Interface conditions depend on the geometry of the interface, the shape of the incident wave front, and the order of continuity of the material constants. The order of continuity of the material constants is made precise by defining the order of the interface. A surface at which the nth derivatives of the elastic parameters are discontinuous is called an interface of $(n+1)$th order. A first-order interface will have discontinuous elastic parameters across it.

For the zeroth order approximation and a smooth first order interface, it is found that the usual results such as Snell's law at planar interfaces apply to a curved interface provided that the principal radii of curvature are large compared with the wavelength in question. More precisely,

(1) when a P or SV wave strikes a first-order interface, only reflected and refracted P and SV waves can appear,

(2) when a SH wave strikes a first order interface, only reflected and refracted SH waves can appear,

(3) the reflection and transmission coefficients of the principal components of the waves are independent of the curvatures, the interface, and the wave front. Moreover, they are dependent on the angle of incidence and the material parameters at the point of incidence.

This requires the tracking of the interfaces relative to the ray paths, the application of Snell's law, and the calculation of mode-converted waves.

4.5. *Boundary Value Problem Formulation*

If it is required that the ray passes through both the source and receiver, then a two-point boundary value problem formulation is, in principle, more suitable. This formulation solves the ray tracing Eq. (4.12) using the τ travel time coordinate or Eq. (4.14) using the arc length coordinate. The boundary conditions for Eq. (4.12) or (4.14) are

$$x_i(0) = x_i^0, \qquad x_i(S) = x_i^s, \quad i = 1, 2, 3. \tag{4.16}$$

Note that the total length along the ray path S is an unknown quantity. Thus, it would seem that the solution is undetermined. A closer examination reveals that the

number of conditions is appropriate for a proper formulation of the two point boundary value problem. The solution of (4.14) and (4.16) is

$$S \qquad \text{and} \qquad x_i(\{x_j^0\}, \{x_j^s\}), \quad i, j = 1, 2, 3.$$

To explicitly display the total length along the ray S, we define

$$s = S\eta \qquad \text{so that} \quad 0 < \eta < 1.$$

Equations (4.14) and (4.16) become

$$\begin{aligned} \frac{dx_i}{d\eta} &= Sv(\mathbf{x})\, p_i, \\ \frac{dp_i}{d\eta} &= S \frac{\partial}{\partial x_i}\left(\frac{1}{v}\right), \qquad 0 < \eta < 1, \\ x_i(0) &= x_i^0, \qquad x_i(1) = x_i^s, \quad i = 1, 2, 3, \end{aligned} \tag{4.17}$$

and

$$\mathbf{x} = (x_1, x_2, x_3).$$

Here, (4.17) is actually a nonlinear eigenvalue problem since the total length S of the ray must be such that the Dirichlet boundary conditions at $\eta = 0$ and $\eta = 1$ are satisfied. This point is clearly recognized by Pereyra *et al.* [75] and is missed by Julian and Gubbins [48]. Consequently, the comparison by Julian and Gubbins of the efficiencies of the shooting and nonshooting methods is invalid.

We may well use the travel time τ as the independent variable and work with Eq. (4.12). This becomes

$$\begin{aligned} \frac{dx_i}{d\xi} &= Tv^2(\mathbf{x})\, p_i, \\ \frac{dp_i}{d\xi} &= -T \frac{\partial}{\partial x_i}(\ln v), \qquad i = 1, 2, 3, \end{aligned}$$

and

$$\tau = T\xi, \qquad 0 < \xi < 1, \tag{4.18}$$

where T is the total travel time along the ray path.

Equations (4.17) or (4.18) may be solved by an initial value technique called the shooting method or by a nonshooting method. The shooting method beings with the integration of the system of first-order ordinary differential equations (4.17), say, with the initial conditions

$$x_i(0) = x_i^0, \qquad i = 1, 2, 3,$$

and some initial estimates of $p_1(0)$, $p_2(0)$, and S. Using the eikonal equation, we have $p_3(0) = \sqrt{(1/v^2(0)) - p_1(0)^2 - p_2(0)^2}$. In terms of $\mathbf{W} = (p_1(0), p_2(0), S)$ the solution at $\eta = 1$ is $x_i(1; \mathbf{W})$, $i = 1, 2, 3$. If $x_i^{(0)}(1; \mathbf{W})$, $i = 1, 2, 3$, satisfy the boundary condition x_i^s, $i = 1, 2, 3$, then $x_i^{(0)}(1; \mathbf{W})$ is a solution of the two-point boundary value problem (4.17). Otherwise, we must modify $p_1(0)$, $p_2(0)$, and S until

$$x_i(1; p_1(0), p_2(0), S) = x_i^s, \qquad i = 1, 2, 3. \tag{4.19}$$

A Newton's method may be used to solve (4.19). Let

$$G_i = x_i(1; \mathbf{W}) - x_i^s.$$

Then Newton's method is stated as

$$J_G(\mathbf{W}_n)(\mathbf{W}_{n+1} - \mathbf{W}_n) = \mathbf{G}(\mathbf{W}_n), \tag{4.20}$$

where

$$J_G(\mathbf{W}) = \begin{bmatrix} \dfrac{\partial x_1}{\partial W_1} & \dfrac{\partial x_2}{\partial W_1} & \dfrac{\partial x_3}{\partial W_1} \\ \dfrac{\partial x_1}{\partial W_2} & \dfrac{\partial x_2}{\partial W_2} & \dfrac{\partial x_3}{\partial W_2} \\ \dfrac{\partial x_1}{\partial W_3} & \dfrac{\partial x_2}{\partial W_3} & \dfrac{\partial x_3}{\partial W_3} \end{bmatrix}. \tag{4.21}$$

To calculate the elements of the Jacobian $J_G(\mathbf{W})$, we solve a set of variational problems obtained by differentiating the boundary value problem (4.17) with respect to W_i, $i = 1, 2, 3$. The total number of differential equations to be integrated simultaneously is 24, eighteen of which are linear. The total number may be reduced by four. However, the coefficients of the equations become complicated. Here, the trade-off is a simpler function evaluation for a larger system of equations.

Alternatively, the boundary value problem (4.17) or (4.18) may be solved by methods for general two-point boundary value problems. These methods satisfy the boundary conditions at each iteration but not the differential equation. It is, therefore, necessary to solve a large system of linear algebraic equations. The essential elements of a two-point boundary problem solver are (1) quasi-linearization to reduce the nonlinear system to a linear one, (2) solution of the resultant linear two-point boundary value problem either by some hybrid scheme or by a discrete coordinate method, i.e., finite differences, or finite elements, and (3) solution of a linear system of equations to obtain the Newton corrections. The quasi-linearization step is a Newton's method in function space.

Julian and Gubbins [48] call this the "bending ray" method. Graphically, we see

that an initial guess at the true ray path between the source and receiver is successively altered by a Newton's iterative scheme to achieve the true ray path. We may use finite differences to solve the linear two-point boundary problem. On the other hand, if we use a finite element method, it is more efficient to begin with a variational statement of the problem based on Fermat's principle.

The steps (1) and (2) may be permuted in sequence. The nonlinear differential equations are discretized first, followed by a method for solving the resultant system of nonlinear algebraic equations. Any of a number of effective nonlinear equation solution methods may be applied here.

4.6. *Ray Amplitude Calculations*

When the response due to a disturbance is needed, the ray amplitudes are calculated along with the ray paths. The main ingredient in a ray amplitude computation is the geometric divergence factor of a ray tube

$$\frac{J(\tau_0)\,\rho(\tau_0)\,v(\tau_0)}{J(\tau)\,\rho(\tau)\,v(\tau)}.$$

Here, $J(\tau)$ is the Jacobian of transformation from the Cartesian coordinates into the "ray coordinates." The ray coordinates are the parameters characterizing a ray. It is seen from our earlier discussion that the triplet (s or τ, p_1^0, p_2^0) completely specifies a ray. The solution is given by either

$$x_i = x_i(s, p_1^0, p_2^0)$$

or

$$x_i = x_i(\tau, p_1^0, p_2^0).$$

The Jacobian $J(\tau)$ of the transformation has a simple form

$$\left| \frac{\partial \mathbf{x}}{\partial p_1^0} \times \frac{\partial \mathbf{x}}{\partial p_2^0} \right|,$$

where $\times$ indices the cross product of two vectors $\mathbf{a} \times \mathbf{b}$, and $|\mathbf{c}|$ is the magnitude of the vector $\mathbf{c}$. Using a Laplace expansion formula, we obtain

$$J(\tau) = \left(\frac{\partial x_i}{\partial p_1^0}\frac{\partial x_i}{\partial p_1^0}\right)\left(\frac{\partial x_j}{\partial p_2^0}\frac{\partial x_j}{\partial p_2^0}\right) - \left(\frac{\partial x_i}{\partial p_2^0}\frac{\partial x_j}{\partial p_2^0}\right)^2. \tag{4.22}$$

There are three methods for estimating $J(\tau)$:

(I) Trace a set of rays and compute the distance between adjacent rays.

(II) Derive differential equations for the elements

$$\frac{\partial x_i}{\partial p_1^0} \quad \text{and} \quad \frac{\partial x_i}{\partial p_2^0}, \qquad i = 1, 2, 3,$$

and evaluate Eq. (4.22).

(III) Solve the differential equations for the Jacobian J.

The differential equations for the elements

$$\frac{\partial x_i}{\partial p_j^0}, \qquad i = 1, 2, 3, \quad \text{and} \quad j = 1, 2,$$

are exactly the variational equations in the shooting method. Therefore, the use of the shooting method for tracing a ray between the source and the receiver gives the ray path and the ray amplitude. Similarly, in the nonshooting method, this information is contained in the Jacobian of Newton's method and, therefore, the ray amplitude may be evaluated with one additional straightforward calculation at the termination of the ray tracing routine. This is indeed a desirable feature of the two-point boundary value methods.

For the initial value methods, we use either scheme (I) or (III). Method (I) is just the procedure of Section 4.5, tracing a ray through a source and a receiver. Since the procedure of Section 4.5 is a variant of a two-point boundary value problem, the ray path and the zeroth approximation of the ray amplitude are simultaneously calculated.

Method (III) is entirely different. Much attention has been focused on deriving the differential equation for J, the Jacobian of the transformation from the Cartesian coordinate to the ray coordinate (see Červený and Hron [14] for a discussion). Červený and Pšenčík [17] derived a set of five first-order differential equations for quantities useful in the computation of J. This set may be further reduced to three nonlinear first order differential equations. More recently, Červený and Hron [14], using a ray centered coordinate, obtain a system of three nonlinear Riccati equations called dynamic ray tracing equations.

4.7. *Comments on Numerical Solution*

For ray tracing applications, it is likely that the ODE system is nonstiff. Therefore, variable-order Adams methods are recommended, as they dynamically adapt the order of integration to the solution behavior. The solvers may be further modified to suit a specific class of problems. This can increase efficiency. For example, computations on a vector machine using a generic Adams method should be vectorized to take advantage of the simplicity of the scheme. The cost of an Adams integration step depends on the costs of evaluating $f(x, y)$ in the ODE system $y' = f(x, y)$. By vectorizing ray tracing problems with the same source location but a set of takeoff angles, we gain computational efficiency since the function evaluations may be performed in parallel.

Another point worth noting is the computation of the ray amplitudes. Here, there are two choices: (1) compute a set of rays with identical initial position but with varying takeoff angles and use this result to obtain the Jacobian of transformation J from the Cartesian coordinates into the ray coordinates or (2) solve simultaneously the five or six ray tracing equations and the three nonlinear or five linear dynamic ray tracing equations for the Jacobian J and the ray path. The first choice has a very simple function to evaluate. In contrast, the dynamic ray tracing equations require an extensive computation to produce the coefficients of the equations. This involves the calculation of the tangent vector t to the ray and two mutually orthogonal vectors e_1 and e_2 to form a basis. This is followed by a transformation to the ray centered coordinate system t, e_1, and e_2, where e_1 and e_2 are aligned with the polarizations of the shear waves. Finally, the coefficients of the dynamic ray tracing equations in the ray centered coordinate system are obtained. This added complexity can negate the gain in the direct computation of the Jacobian J. The trade-off, in using either choice (1) or (2), is that method (1) is more efficient but the Jacobian J may not be as accurate as method (2). The inaccuracy arises from using difference approximations to the derivatives. This question of computational accuracy and efficiency has been ignored by Červený and Hron [14] and requires further in-depth study to settle it.

Next, we turn to the question of ray tracing using a two-point boundary value problem formulation. Here, it is required that the ray path must pass through the source and the receiver. The discussion on solving problems of this sort suggests that the process is expensive as compared with a strictly initial value problem formulation. The initial value problem formulation yields ray paths ignoring the receiver location.

4.8. *Ray Tracing by Circular Approximation*

An approximate method called the "circular approximation" has been proposed for solving the ray tracing equation in two spatial dimensions (Pedersen and Gordon [72], Pedersen [73], Marks [62]). The circular approximation method begins by partitioning the x–z domain Ω into a union of triangles A_k called a grid. Then the velocity field $v(x, z)$ is approximated in each A_k by a piecewise linear approximation

$$v(x, z) = a_k + b_k x + c_k z, \qquad x, z \in A_k.$$

The resultant ray tracing equations in A_k may be solved exactly with the ray path tracing out an arc of a circle. Starting at the triangle containing the source, we trace the ray as a circular path to a side of the triangle. The values of x and z at the intersection point are the initial values for ray tracing solutions on the next triangle. This process is continued onto other triangular subdomains. Curvilinear interfaces may be treated without difficulty.

This method, however, lacks a theoretical foundation. The choice of a grid is very important. This point has been totally neglected. Calculations by Marks [62] indicate that the method is effective and, moreover, the computation of the ray amplitude is simple. Nevertheless, without a rational algorithm for developing the grid, ray tracing

by the circular approximation is but an ad hoc procedure. It would be vauable to have an error analysis developed for this method.

A similar numerical method for solving second-order stiff two-point boundary value problems has been studied by Chin and Krasny [24]. The procedure involves solving differential equations by approximating terms of the equation. The essential ideas are (1) to approximate certain terms of the differential equation over local domains so that the resultant differential equations are easily solved, (2) to apply approximation theory to develop an adaptive mesh strategy, and (3) to patch the local solutions to obtain a global solution.

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