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3D MODELLING OF WAVE PROPAGATION IN SOLID MEDIA AND APPLICATIONS IN GEOPHYSICS

Georgi Boyadzhiev

Abstract. In this paper the geometrical properties of the bi-characteristic curves are employed in developing a new approach to 3D modelling of elastic piecewise homogeneous media, in particular Earth crust and upper Mantle. The method is based on tomography and the refraction, respectively, reflection, of the bi-characteristic curves at the layer boundaries of multi - layered media.

1. Introduction

The aim of this paper is introduction of a new approach to 3D modelling of elastic piecewise homogeneous media, in particular of Lithosphere - Earth crust and upper Mantle. The method is based on classical tomography and the main source of information are seismic waves, generated by a point source S and recorded by a set of seismic stations on the surface of Earth. Irregularity of earthquakes is counterpoised by the density of seismic stations and plenty of data are available for geophysical surveys.

In many contemporary models Earth is considered as an elastic body that is a continuum, in other words the matter is continuously distributed in space. Furthermore, since seismicity has relatively local effect, the planet can be approximated with no loss of generality by the half-space $\Omega = \{(x, y, z) \in R^3 : z \geq 0\}$

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with free surface boundary $\{z = 0\}$ and axis z is positive downword. If the elastic parameters depend only on vertical coordinate z then the wave propagating in solid media satisfy the following strongly coupled linear hyperbolic system (see [1] and [5])

$$
\begin{aligned}
\rho\frac{\partial^2 u_x}{\partial t^2} &= \rho X + (\lambda+2\mu)\frac{\partial^2 u_x}{\partial x^2} + \mu\frac{\partial^2 u_x}{\partial y^2} + \mu\frac{\partial^2 u_x}{\partial z^2} \\
&\quad +(\lambda+\mu)\frac{\partial^2 u_y}{\partial x\partial y} + (\lambda+\mu)\frac{\partial^2 u_z}{\partial x\partial z} + \frac{\partial\mu}{\partial z}\frac{\partial u_x}{\partial z} + \frac{\partial\mu}{\partial z}\frac{\partial u_z}{\partial x} \\
\rho\frac{\partial^2 u_y}{\partial t^2} &= \rho Y + \mu\frac{\partial^2 u_y}{\partial x^2} + (\lambda+2\mu)\frac{\partial^2 u_y}{\partial y^2} + \mu\frac{\partial^2 u_y}{\partial z^2} \\
&\quad +(\lambda+\mu)\frac{\partial^2 u_x}{\partial x\partial y} + (\lambda+\mu)\frac{\partial^2 u_z}{\partial y\partial z} + \frac{\partial\mu}{\partial z}\frac{\partial u_y}{\partial z} + \frac{\partial\mu}{\partial z}\frac{\partial u_z}{\partial y} \\
\rho\frac{\partial^2 u_z}{\partial t^2} &= \rho Z + \mu\frac{\partial^2 u_z}{\partial x^2} + \mu\frac{\partial^2 u_z}{\partial y^2} + (\lambda+2\mu)\frac{\partial^2 u_z}{\partial z^2} \\
&\quad +(\lambda+\mu)\frac{\partial^2 u_x}{\partial x\partial z} + (\lambda+\mu)\frac{\partial^2 u_y}{\partial y\partial z} \\
&\quad +\frac{\partial\lambda}{\partial z}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}\right) + 2\frac{\partial\mu}{\partial z}\frac{\partial u_z}{\partial z}
\end{aligned}
\tag{1}
$$

where λ, μ and ρ are piecewise continuous functions of z and $u_x, u_y, u_z, \sigma_{zz}, \sigma_{zx}$ and σ_{zy} in $C(\Omega)$. Function $u = (u_x, u_y, u_z)$ is called in physics "displacement function".

The boundary conditions of system (1) at the free surface $z = 0$ are

$$
\begin{aligned}
\sigma_{zz} &= (\lambda+2\mu)\frac{\partial u_z}{\partial z} + \lambda\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) = 0 \\
\sigma_{zx} &= \mu\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) = 0 \\
\sigma_{zy} &= \mu\left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right) = 0
\end{aligned}
\tag{2}
$$

Initial data are given by

$$u(S)|_{t=0} = \delta, \frac{du}{dt}(S)|_{t=0} = c.\xi^0 \tag{3}$$

i.e. at the point source $S \in \Omega$ there is an impulse alongside given vector $\xi^0 = (\xi_1^0, \xi_2^0, \xi_3^0)$.

Coefficients ρ, λ and μ depend on the geological properties of the rock. One reasonable approximation of the Lithosphere is 3-dimensional structure of homogeneous blocks in welded contact $\{B_{i,j,k}\}$, where i and j are integers, and k is a natural number. Blocks $B_{i,j,k}$ may be not rectangular ones or their sides may be not parallel to coordinate axis. Without loss of generality we assume the boundary $\partial B_{i,j,k}$ to be piecewise smooth surface and the source S of the seismic signal is in block $B_{0,0,0}$.

This way in $\Omega = \{B_{i,j,k}\}$ the system (1) with constant coefficients in every block $B_{i,j,k}$ is a realistic approximation to the wave propagation in the Lithosphere.

Solving system (1), (2), (3) numerically is limited by some natural constrains as the size the domain Ω. If is not relatively small, that is the general case, the grid is too large and computational time is too costly or the approximation error - too high. On the other hand the fundamental solution of (1) can be explicitly written in integral form since so called Rayleigh and Love modes give good approximation of the solution when the distance from the source is large enough compared to the wavelenght (see [1]). Numerical computing of the integral faces the same problems as pure numerical methods solving (1), (2), (3) directly - the cost of computations and error ratio.

In another standard analytical approach widely used in geophysics, if the body forces are neglected, the solutions of (1) are considered as a plane harmonic waves propagating along the positive x axis

$$u(x,t) = F(z).e^{i(\omega t - kx)},$$

where ω is the angular frequency and k is the wavenumber corresponding to the phase velocity c, i.e. $k = \omega/c$. (see for instance [5]). The main disadvantage of this approach is that the plane wave is two - dimensional one, living in the plane $y = 0$ only, and all information on y coordinate is lost. Therefore it is imposible to build reasonable 3D model using plane wave of such type, which is the reason a new approach for 3-D modeling is suggested in this paper. Since earthquake generates a singularity at point S, the method suggested is builded on the propagation of singularities of system (1) itself.

There are alternative points of view to wave propagating in multi - layered solid media. For instance, In [7] are studied evolution systems for paraxial equations with non-smooth equations that are applied in reflection seismic imaging. Solutions for Cauchy problem of a system with low regularity of the coefficients are given in integral form. In our paper is adopted completely different way to the problem - so called "train" solutions, i.e. the solution in one block determines the boundary conditions of neighbouring blocks.

System (1) in Ω has step - wise coefficients and the classical results for the wave front set (Theorem 8.3.1, [2], v. I, p.271) are not applicable. Hence we use "train solutions" construction in our model. Since the point source $S \in B_{0,0,0}$ in this block we consider initial value problem for system (1) and the initial data (3) determine the solution of system (1) in block $B_{0,0,0}$, as well as on $\partial B_{0,0,0}$. Welded contacts of neighbouring blocks means that solution of (1), (3) on $\partial B_{0,0,0}$ gives the boundary conditions in the neighbouring block and so on. In fact we consider initial value problem for block $B_{0,0,0}$ and boundary valued problems for all other blocks. This way instead if system (1) with piece - wise constant coefficients we consider a series of related problems (1) with constant coefficients, which is much easier task.

This method is based on the features of the bicharacteristic curves of system (1). As the principal part is real with constant coefficients, the wavefront set is invariant under the bicharacteristic flow. Having in mind the source model described above, a point source with seismic impulse in some direction, actually the singularities of the solution carry all the information about the wave. On the other hand, the singularities propagate over bicharacteristic curves within every homogeneous block. At the boundary between two block bicharacteristics could be reflected or refracted. According to geometrical optics and microlocal analysis, if bicharacteristic curve reflects off the sides of every block the angle of incidence to the surface is equal to the angle of reflection. As for refraction at the surface, it is computed in the usual way, more details and exact coputations are given in Chapter 1 below. Therefore, if we know the position of the source S, the direction ξ_0 of the seismic impulse and media structure $\Omega = \{B_{i,j,k}\}$ we can compute the intersecting point s_0 of the bicharacteristic curve and the surface z=0. The point s_0 is in fact the centre of the surface waves in the plane z=0 generated by the section of the wave front and the plane z=0. When actual measurement of the seismic waves is done, the coordinates of the point s_0 can be triangulated using the data from several stations. This way verification of the media model $\Omega = \{B_{i,j,k}\}$ is done. Exact coordinates of the epicenter of an eqrthquake and the centre of the surface waves r_0 is computed using different and quite reliable techniques, like time - frequency analysis, based on the data from seismic stations. Geven a certain 3-D media model $\Omega = \{B_{i,j,k}\}$, we compute the point s_0. If the points s_0 and r_0 coincide within the error of the computations, then the media model is plausible. For practical purposes 3-D models $\Omega = \{B_{i,j,k}\}$ are generated using Monte Carlo type methods. Of course, like any other inverse problem, this algorithm has multiple solutions in the sense that many models can fulfill the requirement $s_0 = r_0$.

2. Characteristic set and bicharacteristic strip in homogeneous blocks $B_{i,j,k}$

Let $L_{k,m}(x, D) = \sum_{|\alpha|\leq 2} a_\alpha^{k,m}(x)D^\alpha$. Then the characteristic set of linear strongly coupled system

$$\sum_{m=1}^{n} L_{k,m}(x, D)u_m = f_i, k = 1, ...n$$

is given by $det|p_{k,m}(x, \xi)| = 0$ where $p_{k,m}(x, \xi) = \sum_{|\alpha|=2} a_\alpha^{k,m}(x)\xi_m^\alpha$ (see [6], p.40).

If we denote by $\alpha = -(\lambda+\mu)^{-1}\left[\rho\tau^2 - \mu\left({\xi_1}^2 + {\xi_2}^2 + {\xi_3}^2\right)\right]$, the characteristic set of system (1) in every the block $B_{i,j,k}$ is given by the equation

$$0 = \begin{vmatrix} \alpha + {\xi_1}^2 & \xi_1\xi_2 & \xi_1\xi_3 \\ \xi_1\xi_2 & \alpha + {\xi_2}^2 & \xi_2\xi_3 \\ \xi_1\xi_3 & \xi_2\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} =$$

$$= \alpha \begin{vmatrix} \alpha + {\xi_2}^2 & \xi_2\xi_3 \\ \xi_2\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} + \begin{vmatrix} {\xi_1}^2 & \xi_1\xi_2 & \xi_1\xi_3 \\ \xi_1\xi_2 & \alpha + {\xi_2}^2 & \xi_2\xi_3 \\ \xi_1\xi_3 & \xi_2\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} =$$

$$= \alpha \begin{vmatrix} \alpha + {\xi_2}^2 & \xi_2\xi_3 \\ \xi_2\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} + \alpha \begin{vmatrix} {\xi_2}^2 & \xi_1\xi_3 \\ \xi_1\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} + \begin{vmatrix} {\xi_1}^2 & \xi_1\xi_2 & \xi_1\xi_3 \\ \xi_1\xi_2 & {\xi_2}^2 & \xi_2\xi_3 \\ \xi_1\xi_3 & \xi_2\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} =$$

$$= \alpha \begin{vmatrix} \alpha + {\xi_2}^2 & \xi_2\xi_3 \\ \xi_2\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} + \alpha \begin{vmatrix} {\xi_1}^2 & \xi_1\xi_3 \\ \xi_1\xi_3 & \alpha + {\xi_3}^2 \end{vmatrix} + \begin{vmatrix} {\xi_1}^2 & \xi_1\xi_2 \\ \xi_1\xi_2 & {\xi_2}^2 \end{vmatrix} + \begin{vmatrix} {\xi_1}^2 & \xi_1\xi_2 & \xi_1\xi_3 \\ \xi_1\xi_2 & {\xi_2}^2 & \xi_2\xi_3 \\ \xi_1\xi_3 & \xi_2\xi_3 & {\xi_3}^2 \end{vmatrix} =$$

$$= \alpha^2\left(\alpha + {\xi_1}^2 + {\xi_2}^2 + {\xi_2}^2\right).$$

These simple calculations show that the characteristic set of system (1) consists of two subsets

$$p_1(x,\xi) = \rho\tau^2 - \mu\left({\xi_1}^2 + {\xi_2}^2 + {\xi_3}^2\right) = 0 \tag{4}$$

$$p_2(x,\xi) = \rho\tau^2 - (\lambda + 2\mu)\left({\xi_1}^2 + {\xi_2}^2 + {\xi_3}^2\right) = 0$$

since $(\lambda + \mu) > 0$.

Therefore the wave propagating in homogeneous block $B_{i,j,k}$ is actually a composition of two waves. This result corresponds to the theory of P (primary) and S (secondary) body waves. P wave corresponds to the set defined by $p_2(x,\xi) = 0$, and S wave - to the one defined by $p_1(x,\xi) = 0$.

Hence the following theorem holds:

Theorem 1. *Body wave propagating in homogeneous block $B_{i,j,k}$ is composition of two waves - P wave and S wave. There are no other components of the wave.*

The charecteristic set of an operator contains the wave front of the solution u (see [2], vol. I, Theorem 8.3.1, p.271). Roughly speaking, the wave front of u is a conic set where u is not smooth (see [2], Def. 8.1.2 p.254). In terms of physics the wave front describes the position of the wave at the moment.

Furthermore, the characteristic set of a operator with real principal part $p(x,\xi)$ and constant coefficients is invariant under the bicharacteristic flow (see [2], vol. I, Chapter 8). The restriction of the bicharacteristic strip into R^4 is named bicharacteristic curve. It is applicable to 3D modeling of the Earth, for, generally speaking, the singularities propagate over the bicharacteristic curves. In other words, singularity that is generated by an earthquake in block $B_{0,0,0}$ propagate over the bicharacteristic curve in $B_{0,0,0}$ untill it intersects at point (x_1, y_1, z_1) the boundary to the neighbouring block, $B_{1,0,0}$ for instance. Continuous boundary conditions meen that at point (x_1, y_1, z_1) system (1) in the block $B_{1,0,0}$ has singularity, that propagates over the bicharacteristic curves in $B_{1,0,0}$, etc.

By definition if $p(x^0, \xi^0) = 0$ then the bicharacteristic strip at point (x^0, ξ^0) is defined by the Hamilton equations

$$\frac{dx}{ds} = \frac{\partial p(x,\xi)}{\partial \xi}, \frac{d\xi}{ds} = \frac{\partial p(x,\xi)}{\partial x}$$

with initial data $(x,\xi) = (x_0, \xi_0)$ for $t = 0$. The corresponding bicharacteristic curve is

$$(5) \qquad \left| \begin{array}{l} x_1 = c^{-1}\xi_1^0.(t-t^0) + x_1^0 \\ \\ x_2 = c^{-1}\xi_2^0.(t-t^0) + x_2^0 \\ \\ x_3 = c^{-1}\xi_3^0.(t-t^0) + x_3^0 \end{array} \right|$$

since $t - t^0 = 2c\sqrt{(\xi_1^0)^2 + (\xi_2^0)^2 + (\xi_3^0)^2}.s = 2c|\xi^0|$ and without loss of generality we may assume $|\xi^0| = 1$. Constant $c = \sqrt{\mu/\rho}$ for bicharacteristics generated by $p = p_1(x,\xi)$ and $c = \sqrt{(\lambda+2\mu)/\rho}$ for ones generated by $p = p_2(x,\xi)$.

The values of ξ_1^0, ξ_2^0 and ξ_3^0 are determined by the features of the seismic source. Without loss of generalization we can assume source of the seismic wave to be a point one with direction of the impulse $\xi_1^0, \xi_2^0, \xi_3^0$.

3. Reflection and refraction

Equation (5) describes the bicharacteristic curves of (1) in each $B_{i,j,k}$ and their behavior on the boundary $\partial B_{i,j,k}$ is studied by geometrical optics and microlocal analysis.

Let b^{in} be a bicharacteristic curve in $B_{i,j,k}$ and $b^{in} \cup \{F_{i,j,k,l}(x,y,z) = 0\} = p_0$. At point p_0 b^{in} can be reflected or refracted. Let b_{rr} be the refracted curve and b_{rl} be the reflected one. Both b_{rr} and b_{rl} are bicharacteristics through point p_0 - b_{rr} is in the next to $B_{i,j,k}$ block (in the sense of propagation of the singularity generated in S) and b_{rl} is in $B_{i,j,k}$. The singularity at p_0 propagates over the bicharacteristics as well and this way the well - known following formula for reflection and refraction from geometrical optics are obtained.

If incidental bicharacteristic curve b^{in} is reflected the angle θ_{in} of incidence to the surface $F_{i,j,k,l}(x,y,z) = 0$ is equal to the angle of reflection θ_{rl}, since in the same block the equation (5) has the same coefficients. As for refraction at a surface, the match of the boundary conditions of the neighbouring blocks at the two sides of the boundary lead to the well - known formula from geometric optics $v_1 \sin\theta_{rr} = v_2 \sin\theta_{in}$, where θ_{rr} is the angle of refraction, v_1 is the speed of the wave in the "incidence" block and v_2 is the one in "refraction" block.

Computation of reflected and refracted bicharacteristic curve is simple. Let $\vec{n} = (n_1, n_2, n_3) = \left[\left(\frac{\partial F}{\partial x}\right)^2 + \left(\frac{\partial F}{\partial y}\right)^2 + \left(\frac{\partial F}{\partial z}\right)^2\right]^{-1/2} \left(\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y}, \frac{\partial F}{\partial z}\right)(p_b)$ be the normal unit vector to surface $F_{i,j,k,l} = 0$ at the point of incidence p_b, $\xi^{in} = (\xi_1^{in}, \xi_2^{in}, \xi_3^{in})$ be the unit vector along the incidental bicharacteristic curve, $\xi^{rr} =$

$(\xi_1^{rr}, \xi_2^{rr}, \xi_3^{rr})$ be the unit vector along refracted one, and $\xi^{rl} = \left(\xi_1^{rl}, \xi_2^{rl}, \xi_3^{rl}\right)$ be the unit vector along reflected one.

The speed of the wave is a physical feature of every material and it is preliminary known. For instance, the velocity of the P-wave in homogeneous isotropic medium is $v_P = \sqrt{(\lambda + 2\mu)/\rho}$, for S-wave it is $v_S = \sqrt{\mu/\rho}$.

Quantities $\sin\theta_{in} = \sin\theta_{rl}$ and $\sin\theta_{rr}$ are easy to compute using scalar, or dot product $\cos\theta = \xi \cdot \vec{n}$ of unit vectors ξ and the normal unit vector $\vec{n}$, for instance

$$\sin^2\theta_{in} = 1 - \left(\xi_1^{in} n_1 + \xi_2^{in} n_2 + \xi_3^{in} n_3\right)^2$$

Then equations of refraction and reflection from geometrical optics yield

$$\begin{aligned} \xi_1^{rr} n_1 + \xi_2^{rr} n_2 + \xi_3^{rr} n_3 &= \left[1 - \left(\frac{v_2}{v_1}\right)^2 \left(1 - [\xi_1^{in} n_1 + \xi_2^{in} n_2 + \xi_3^{in} n_3]^2\right)\right]^{1/2} \\ \xi_1^{rl} n_1 + \xi_2^{rl} n_2 + \xi_3^{rl} n_3 &= \left[1 - \left(1 - [\xi_1^{in} n_1 + \xi_2^{in} n_2 + \xi_3^{in} n_3]^2\right)\right]^{1/2} \end{aligned} \tag{6}$$

In addition, the incidental bicharacteristic curve, the refracted one and the normal to the surface vector lie on the same plane and give us the relation

$$\begin{vmatrix} n_1 & n_2 & n_3 \\ \xi_1^{in} & \xi_2^{in} & \xi_3^{in} \\ \xi_1^{rr} & \xi_2^{rr} & \xi_3^{rr} \end{vmatrix} = 0. \tag{7}$$

The same relation is valid for vector ξ^{rl}.

Finally, since we consider vectors ξ^{in}, ξ^{rr} and ξ^{rl} be unit ones, we obtain

$$\begin{aligned} (\xi_1^{rr})^2 + (\xi_2^{rr})^2 + (\xi_3^{rr})^2 &= 1 \\ (\xi_1^{rl})^2 + (\xi_2^{rl})^2 + (\xi_3^{rl})^2 &= 1 \end{aligned} \tag{8}$$

Equations (6), (7) and (8) define uniquely vectors of refraction ξ^{rr} and reflection ξ^{rl} up to the sigh.

4. 3-D modeling of Earth crust and upper mantle

Using bicharacterstic curves, described in the previous section, it is possible to define the following criterion for 3D model of the Earth crust and upper mantle.

Definition 1. *Let $\{B_{i,j,k}\}$ be a set of blocks and the source of seismic wave be a point one at the point S with direction alongside vector ξ^0. Let P is the point of the Earth surface belonging to the bicharacteristic curves generates by system (1), set of blocks $\{B_{i,j,k}\}$ and source S. Given set of blocks $B_{i,j,k}$ is plausible if the point P coincides with the epicenter E of the surface waves generated by the earthquake.*

Since seismic stations record both surface and body waves, point E is a subject of triangulation if there are enough sensors in the region.

Computing the bi-characteristic curves in all set $\{B_{i,j,k}\}$ arises an important question. At the boundaries between two blocks - surfaces $F_{i,j,k,l}(x, y, z) = 0$ - is the bicharacteristic curve reflected, refracted, or both? The answer comes from so - called reflection and refraction index. It is a physical feature of the material that build the block. How to compute refraction and reflection index is well described in Aki and Richards (2002), W.M. Ewing, W. S. Jardetzky, F. Press. (1957) or in W. L. Plant (1979).

Furthermore, the body waves records are useful to determine the block structure of the closest to the seismic stations blocks. Wave front in a homogeneous block is a subset of the characteristic set of system (1), therefore it has constant speed by (4).

Using bi-characteristic curves and the characteristic set we can compute arrival time for P - and S - waves. In combination with the criteria from the Definition, we can generate and test plausible 3-D models of the Earth crust and upper mantle.

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Georgi Boyadzhiev
Institute of Mathematics and Informatics
Acad. G. Bonchev Str. Bl. 8
1113 Sofia, Bulgaria
e-mail: gpb@math.bas.bg