

Estimation of Elastic Wave Velocities in Anisotropic Solids

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Abstract

In this work, a computer program is developed which allows to find and graph the phase velocities, group velocities and the slowness of a solid from its physical characteristics, namely the stiffness tensor and the volumetric density of the material that composes it. The graphs are also made in such a way that it is possible to obtain the magnitudes according to the angle and the coordinate plane of a specific propagation direction, which are given to the program as inputs.

Keywords: Stress, strain, stiffness tensor, Christoffel tensor, phase velocity, group velocity, slowness, polarization vectors

Introduction

We consider a linear behavior between stress σ_{ij} and strain $\epsilon_{k\ell}$,

$$\sigma_{ij} = C_{ijkl}\epsilon_{k\ell}$$

where C_{ijkl} represents the elastic constants and the symmetries of the material. It can be shown that this so-called stiffness tensor never has 81 independent elements due to the following three relations of symmetry, that is,

$$C_{ijkl} = C_{ijlk} \quad (1)$$

$$C_{ijkl} = C_{jikl} \quad (2)$$

$$C_{ijkl} = C_{klij} \quad (3)$$

In the most complex scenario, it has 21 components. That is the case of the triclinic structures. If the crystal has more symmetries, the number of independent constants decreases. Isotropic crystals are the simplest and they only have two constants.

Newton's second law for continuous media states

$$F_i + \sigma_{ij,j} = \rho \ddot{u}_i$$

where F_i are body forces (force per volume) which are assumed to be zero and u_i is the displacement vector. The subscripts after the comma indicate derivatives with respect to space coordinates and the dots above the letters indicate derivatives with respect to time. Using the symmetries of the tensor C_{ijkl} the wave equation for a linear, anisotropic solid is obtained

$$C_{ijkl}u_{k,i\ell} = \rho \ddot{u}_i$$

Harmonic solutions of the form $u_i = A_{0i}e^{i(\vec{k}\cdot\vec{x}-\omega t)}$ are proposed for this equation so the following one is reached:

$$(\Gamma_{ik} - \rho\delta_{ki}c^2)A_{0i} = 0 \quad (4)$$

with Γ_{ik} the so-called Christoffel tensor, which is defined by

$$\Gamma_{ik} = C_{ijk\ell} l_\ell l_j. \quad (5)$$

Γ_{ik} is a symmetric tensor, which is determined by the stiffness tensor and the directions of propagation (Aki and Richards, 1980, Borrelli, 2013).

We deal with a homogeneous system of three equations and three unknowns, which has non-trivial solutions if the determinant of the matrix of coefficients that multiplies the unknowns is zero (Truell et al., 1969, Santaló, 1977).

$$\det(\Gamma_{ik} - \rho \delta_{ki} c^2) = 0$$

where c can be found to make the equation hold. Substituting the velocities found in the system (4), the unknowns A_{0i} are found. The most general case is when we have three waves as the result, one longitudinal P-wave, which has the greatest speed, and two transversals, called S. In some cases, the two S-waves may be the same.

From the velocity, other magnitudes are obtained, which have different applications. When studying, for example, refraction of waves between anisotropic media, velocity c doesn't matter but its reciprocal $m = 1/c$, called "slowness" of the wave, does matter. Its graphical representation on the coordinate planes allows to deduce the angles of a refracting wave, in the most general case, from one anisotropic medium to another. On the other hand, the velocity of a wave propagating in an anisotropic solid depends on the frequency of the wave. The anisotropic solid is then a dispersive medium, and as such, it has phase velocities and group velocities. The velocities of system (4) are phase velocities. Group velocities, on the other hand, are calculated as follows.

$$g_\ell = \frac{C_{ijk\ell} \alpha_i \alpha_k l_j}{\rho c} \quad (6)$$

with $\alpha_i = A_{0i}/A = A_{0i}/\sqrt{A_{0j}A_{0j}}$ the normalized polarization vector that corresponds to the obtained phase velocity, c (Ruzzante, 2020, Davis, 2000).

Development

A web application that graphs the velocities of propagation on the coordinate planes from characteristics of the material was made. The corresponding URL address is <https://www.elasticas.app/>. It is worth noting that all the technologies used for developing the application have open-source licences.

Aspect and use of the application

When entering the URL of the program by means of any web browser, e.g.: Brave, Google Chrome, Mozilla Firefox, Microsoft Edge, etc., a webpage like the one shown on Figure 1 appears. It consists of the elements specifically listed below.

- Input
 - 21 text fields for the components of the stiffness tensor.
 - One text field to enter the density.
 - A drop-down list to apply symmetries to the stiffness tensor.
 - Another drop-down list, for loading materials stored in the program.
- Output
 - Values of the chosen quantities and the polarization vectors.
 - Buttons to choose the magnitude, whose results are going to be shown: phase velocity, group velocity, slowness.
 - Buttons to choose the coordinate plane from which results are going to be expressed.

- Text field to enter the polar angle in degrees, from which results are going to be expressed.

Elastic waves

C = Stiffness matrix (GPa)

0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0

Density $\rho =$ kg/m^3

Symmetry

Material

2D plot

2D plot parameters

Coordinate plane

XY XZ YZ

Angle (°)

Phase velocity (m/s) Slowness (s/m $\times 10^{-5}$) Group velocity (m/s $\times 10^{-7}$)

0 0 0

Polarization vectors (m)

[0 0 0]

[0 0 0]

[0 0 0]

Figure 1: Screenshot of the web application interface as soon as it's loaded.

After loading data in some way like, for example, selecting a material from the drop-down list, velocity curves appear, as well as their values for the given angle, and the polarization vectors for that angle. In Figure 2, the results appear for the “lithium” material, the XY coordinate plane, and the phase velocity as the chosen quantity. The rest of the fields, corresponding to stiffness constants, the density and the symmetry, are filled automatically.

Values at specific angles can be seen as shown in Figure 3. To do so, the angle is entered in the field “Angle” and the Enter key is pressed, or a click is made in the graph to obtain an approximated value.

It should be noted that the angle can be swept continuously if, besides clicking in the graph, the button is held while the mouse is moved over it. This operation updates, also continuously, the values of velocity and the components of the polarization vectors.

Elastic waves

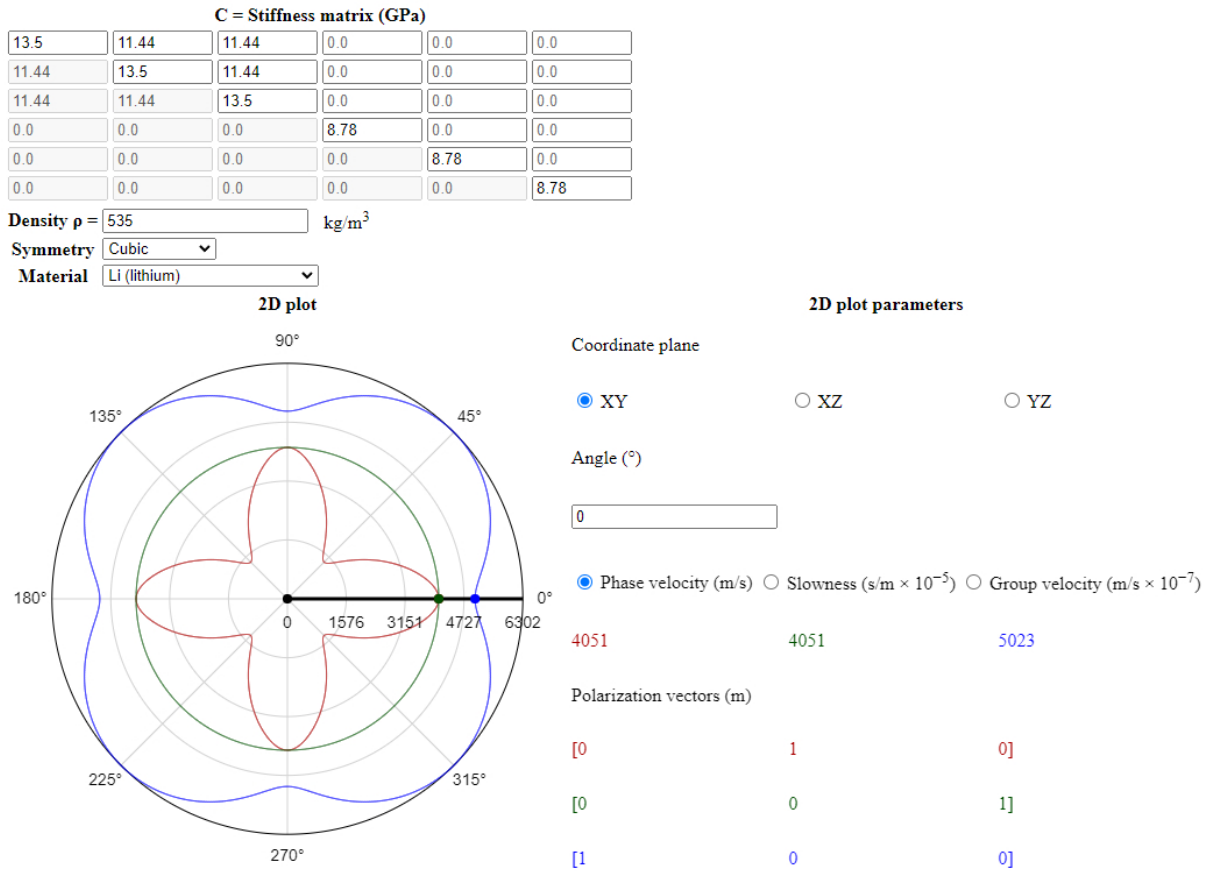


Figure 2: Screenshot of the interface with the results of the lithium.

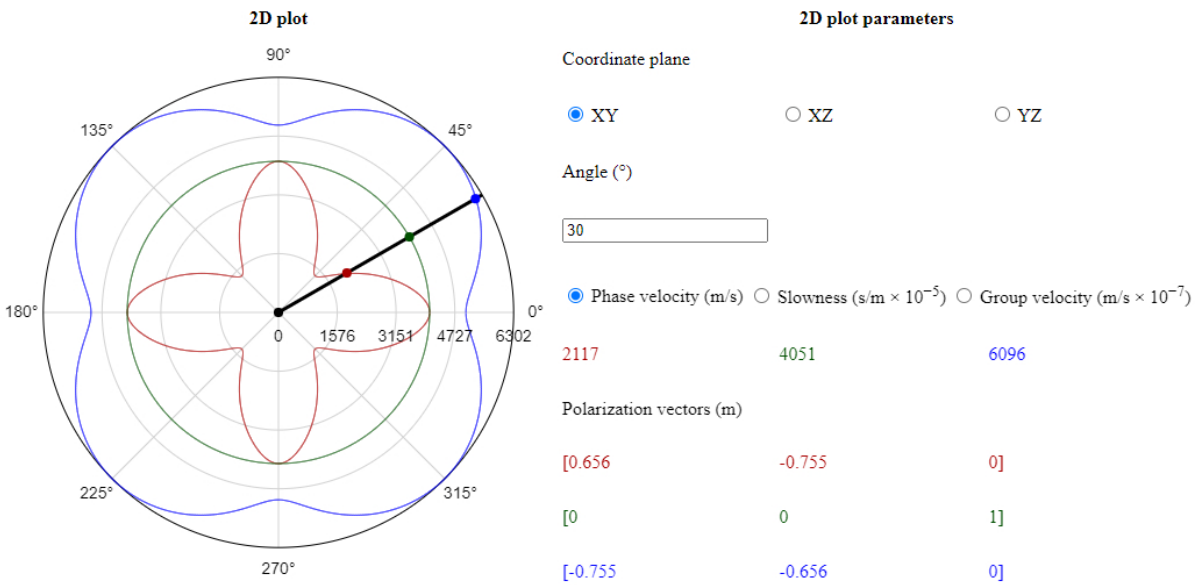


Figure 3: Visualization of the graph and values for an angle of 30°.

Design decisions

The interface was designed under two conditions.

1. The estimation of phase velocity, group velocity, slowness and polarization vectors on the coordinate planes for all angles should be possible.
2. A person with knowledge of waves in anisotropic solids should be able to use it, guided almost entirely by intuition.

The first point states the necessary conditions for the design: the minimum number of elements for entering data and the output elements. The second condition is less objective and, consequently, difficult to address without ambiguities, but it determined the criteria used to add functionalities and make specific decisions.

- Since C is symmetric, offering 36 text fields to fill it is a total design incompetence. The program interface synchronizes the lower and upper triangles automatically, as shown in Figure 4. Only the diagonal and the upper triangle are enabled for writing.
- It is essential to include units next to the elements corresponding to values of physical quantities. It would be much less intuitive to have, for example, the text field of Figure 5, without indicating if the density is expressed in kg/m^3 , g/cm^3 , etc.
- A text field triple was considered to enter a direction of propagation in space and get the results from it. The plot with continuous angle sweep replaced it: it clearly offers a better experience.
- The colors of the plot curves correspond to the results of velocities shown. They also match the colors of the polarization vectors, shown as stacked rows in a matrix. Using colors is not the only possibility, but it is better than nothing and it is what ended up being implemented.

Other issues of importance for a good user experience are the practicality and the compatibility of the application on different systems. They are not issues primarily determined by the interface design, but rather by the selection of software technologies used to create the application.

C = Stiff

0.0	123	0.0
123	0.0	0.0
0.0	0.0	0.0

Figure 4: Text field in the upper triangle being synchronized with its counterpart in the lower triangle.

Density ρ =

Figure 5: Bad example of a text field without units.

Tools

Although developing a desktop application was initially considered, the difficulties encountered in testing the prototype on different computers motivated the passage to the vast, ubiquitous and competitive world of web applications.

The performance of desktop applications is subject to several factors like the operating system, the compilation method or the state of a proper runtime environment, shared libraries, and other dependencies in general. Instead, a web application works in any browser without the need to configure anything or perform additional installations. Another point that was mentioned earlier, without much emphasis, though it is not a minor issue, is the fact that all the tools were chosen in such a way that they had open-source licences. Closed-source tools are more restrictive and not everything that is done with them may be freely published. That limits the scopes of this work, since it has an intrinsically public nature.

With all this in mind, it was decided to use the tools listed below.

- The Python programming language (Python, 2022).
 - The Numpy numerical calculation module (NumPy, 2022).
 - The Flask web server module (Flask Documentation, 2022).
- The PythonAnywhere cloud platform (PythonAnywhere, 2022).
- HTML, CSS and Javascript for the user interface, although technically using them *was not an option*, because they are *standard* (Standards - W3C, 2022).

The list of technologies could be continued recursively, since every language, platform and module in turn depends on other modules. It only highlights that they have open-source licenses, too. The rest of the tools are omitted to avoid unnecessary thoroughness.

Adaptation of expressions

The Numpy numerical calculation module is optimized for matrix operations. It is therefore appropriate to modify the expressions, using matrix representations for their implementation in the software.

Equation (4) amounts to a problem that is solved by finding the eigenvalues and eigenvectors of the matrix of components Γ_{ik} , the Christoffel matrix, which will be denoted $\mathbf{\Gamma}$. This notation passage is valid because the Christoffel tensor is of order two. The same does not hold for the stiffness tensor C_{ijkl} , which is of order four. What it does hold, thanks to the symmetry relations (1), (2) and (3), is the so-called ‘‘Voigt Notation’’. With this notation, the pair of indices of the C_{ijkl} tensor are contracted to two, leading to a tensor C_{pq} . The transformation rules for each pair of indices are the ones that follow:

$$\begin{array}{lll} 11 \rightarrow 1 & 22 \rightarrow 2 & 33 \rightarrow 3 \\ 23 \rightarrow 4 & 13 \rightarrow 5 & 12 \rightarrow 6 \end{array}$$

The components of the stiffness tensor C_{ijkl} can now be represented in a matrix \mathbf{C} as follows:

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix}$$

Each element of the matrix represents more than one element of the tensor due to the symmetry relations (1) and (2). For example, C_{54} may be the representation of C_{1323} as well as C_{1332} or C_{3123} . On the other hand, the components of the lower triangle are equal to the components of the upper triangle, i.e., the matrix \mathbf{C} is symmetric.

$$\mathbf{C} = \mathbf{C}^T \tag{7}$$

This is due to the equality (3). For example, $C_{1323} = C_{2313}$ so using Voigt Notation $C_{54} = C_{45}$. The same goes for the rest of the components: in general, $C_{ijkl} = C_{klij}$ becomes $C_{pq} = C_{qp}$ with Voigt Notation and it turns out that (7) is true.

Voigt Notation is used in this work to replace the tensors of the equation (5) by matrix products, which are easier to implement in a computer program efficiently. For this purpose, the following matrix is defined

$$\mathbf{L} = \begin{bmatrix} l_1 & 0 & 0 \\ 0 & l_2 & 0 \\ 0 & 0 & l_3 \\ 0 & l_3 & l_2 \\ l_3 & 0 & l_1 \\ l_2 & l_1 & 0 \end{bmatrix}$$

and after working on the corresponding sums, each component of the Christoffel tensor is equal to a bilinear form with associated matrix \mathbf{C} . For example, the explicit form of the second row and third column of the Christoffel tensor is

$$\begin{aligned} \Gamma_{23} &= C_{2131}l_1l_1 + C_{2132}l_1l_2 + C_{2133}l_1l_3 \\ &+ C_{2231}l_2l_1 + C_{2232}l_2l_2 + C_{2233}l_2l_3 \\ &+ C_{2331}l_3l_1 + C_{2332}l_3l_2 + C_{2333}l_3l_3 \end{aligned}$$

which using Voigt Notation and symmetries (1), (2) and (3) becomes

$$\begin{aligned} \Gamma_{23} &= C_{65}l_1l_1 + C_{64}l_1l_2 + C_{63}l_1l_3 \\ &+ C_{25}l_2l_1 + C_{24}l_2l_2 + C_{23}l_2l_3 \\ &+ C_{45}l_3l_1 + C_{44}l_3l_2 + C_{43}l_3l_3 \end{aligned}$$

then defining

$$\mathbf{L}_2 = \begin{bmatrix} 0 \\ l_2 \\ 0 \\ l_3 \\ 0 \\ l_1 \end{bmatrix} \quad \mathbf{L}_3 = \begin{bmatrix} 0 \\ 0 \\ l_3 \\ l_2 \\ l_1 \\ 0 \end{bmatrix}$$

as the second and third column of \mathbf{L} respectively, the form becomes

$$\Gamma_{23} = \mathbf{L}_2^T \mathbf{C} \mathbf{L}_3$$

which is the bilinear form that was sought. The same is repeated for the rest of the components and it is finally inferred that

$$\mathbf{\Gamma} = \begin{bmatrix} \mathbf{L}_1^T \mathbf{C} \mathbf{L}_1 & \mathbf{L}_1^T \mathbf{C} \mathbf{L}_2 & \mathbf{L}_1^T \mathbf{C} \mathbf{L}_3 \\ \mathbf{L}_2^T \mathbf{C} \mathbf{L}_1 & \mathbf{L}_2^T \mathbf{C} \mathbf{L}_2 & \mathbf{L}_2^T \mathbf{C} \mathbf{L}_3 \\ \mathbf{L}_3^T \mathbf{C} \mathbf{L}_1 & \mathbf{L}_3^T \mathbf{C} \mathbf{L}_2 & \mathbf{L}_3^T \mathbf{C} \mathbf{L}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{L}_1^T \\ \mathbf{L}_2^T \\ \mathbf{L}_3^T \end{bmatrix} [\mathbf{C}] [\mathbf{L}_1 \quad \mathbf{L}_2 \quad \mathbf{L}_3]$$

so

$$\mathbf{\Gamma} = \mathbf{L}^T \mathbf{C} \mathbf{L}.$$

Symmetry of \mathbf{C} directly implies symmetry of $\mathbf{\Gamma}$ which is easy to see by using equation (7)

$$\mathbf{\Gamma}^T = (\mathbf{L}^T \mathbf{C} \mathbf{L})^T = \mathbf{L}^T \mathbf{C}^T (\mathbf{L}^T)^T = \mathbf{L}^T \mathbf{C} \mathbf{L} = \mathbf{\Gamma}.$$

On the other hand, (6) is worked out for each value of the index ℓ and, with a similar procedure as above, it is proven that the group velocity corresponding to the phase velocity c is

$$\mathbf{g} = \frac{1}{\rho c} (\mathbf{l}^T \mathbf{A}^T \mathbf{C} \mathbf{A})$$