COMPARISON OF RAY METHODS WITH THE EXACT SOLUTION IN THE 1-D ANISOTROPIC "SIMPLIFIED TWISTED CRYSTAL" MODEL

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ABSTRACT

The exact analytical solution for the plane S wave, propagating along the axis of spirality in the simple 1-D anisotropic "simplified twisted crystal" model, is compared with four different approximate ray-theory solutions. The four different ray methods are (a) the coupling ray theory, (b) the coupling ray theory with the quasi-isotropic perturbation of travel times, (c) the anisotropic ray theory, (d) the isotropic ray theory. The comparison is carried out numerically, by evaluating both the exact analytical solution and the analytical solutions of the equations of the four ray methods. The comparison simultaneously demonstrates the limits of applicability of the isotropic and anisotropic ray theories, and the superior accuracy of the coupling ray theory over a broad frequency range. The comparison also shows the possible inaccuracy due to the quasi-isotropic perturbation of travel times in the equations of the coupling ray theory. The coupling ray theory thus should definitely be preferred to the isotropic and anisotropic ray theories, but the quasi-isotropic perturbation of travel times should be avoided. Although the simplified twisted crystal model is designed for testing purposes and has no direct relation to geological structures, the wave-propagation phenomena important in the comparison are similar to those in the models of geological structures.

In additional numerical tests, the exact analytical solution is numerically compared with the finite-difference numerical results, and the analytical solutions of the equations of different ray methods are compared with the corresponding numerical results of 3-D ray-tracing programs developed by the authors of the paper.

Keywords: coupling ray theory, quasi-isotropic approximation, anisotropic ray theory, isotropic ray theory, validity conditions of ray methods

1. INTRODUCTION

In the *isotropic ray theory*, the velocities of both S–wave polarizations are assumed to be equal, which applies to strictly isotropic models only. In the *anisotropic ray theory*, both S–wave polarizations are assumed to be strictly decoupled, which can only be fulfilled in considerably anisotropic models. *Thomson, Kendall and Guest (1992)* demonstrated analytically that the high–frequency asymptotic error of the anisotropic ray theory is inversely proportional to the second or higher root of frequency if a ray pass through the point of equal S–wave eigenvalues of the Christoffel matrix. The *coupling ray theory* (*Coates and Chapman, 1990*) is applicable at all degrees of anisotropy, from isotropic to considerably anisotropic models. The frequency–dependent coupling ray theory is the generalization of both the zero–order isotropic and anisotropic ray theories and provides continuous transition between them. *Pšenčík and Dellinger (2001)* numerically compared the coupling ray theory with the isotropic ray theory, anisotropic ray theory and reflectivity method. One of the simplest models, useful for demonstrating the limits of applicability of the zero–order isotropic and anisotropic ray theories and for testing the coupling ray theory, is the "simplified twisted crystal" model. *Rümpker, Tommasi and Kendall (1999)* numerically compared their coupling ray theory algorithm, based on the "forward propagator method", with the anisotropic ray theory in the case of the plane S wave vertically propagating in several simple 1-D anisotropic models, including the simplified twisted crystal model.

The *"twisted crystal"* model is created of a homogeneous anisotropic elastic material by uniformly helicoidally twisting the x_1x_2 coordinate plane about the x_3 Cartesian coordinate axis. The great advantage of this model is that the exact analytical solution for the plane S wave propagating along the axis of spirality can be derived analytically (*Lakhtakia, 1994*; *Klimeš, 2004*). The general plane–wave solution for the general initial conditions expressed in terms of displacement and stress was derived by *Lakhtakia (1994)*, who also presented explicit analytical equations for the *"simplified twisted crystal"* model with vanishing elastic moduli a_{1333} and a_{2333}, in which the u_1 and u_2 displacement components are strictly separated from the longitudinal u_3 component. *Klimeš (2004)* concentrated on the 2×2 one–way propagator matrices in the simplified twisted crystal model, suitable for comparison with the coupling ray theory.

The simplified twisted crystal model is designed for testing purposes and has no direct relation to geological structures, but the rotation of the eigenvectors of the Christoffel matrix about the ray and the related wave–propagation phenomena are similar to those in the models of geological structures. In the simplified twisted crystal model, the rotation of the eigenvectors of the Christoffel matrix corresponds to the rotation of the crystal axes. In the models of geological structures, the rotation of the eigenvectors of the Christoffel matrix is usually caused by the heterogeneities bending rays rather than by the rotation of the crystal axes.

The main objective of this paper is to demonstrate the applicability and accuracy of the coupling ray theory, of the anisotropic ray theory and of the isotropic ray theory. We compare numerically the exact analytical solution with four different approximate ray–theory solutions. The approximate solutions correspond to the coupling ray theory of *Coates and Chapman (1990)* implemented according to *Bulant and Klimeš (2002)*, to the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation of the coupling ray theory according to *Pšenčík (1998a)* and *Pšenčík and Dellinger (2001)*, and to the zero–order anisotropic and isotropic ray theories. For the exact analytical solution and for the analytical solutions of the equations of the four ray methods, refer to *Klimeš (2004)*.

The numerical comparison of the four ray methods with the exact solution in the simplified twisted crystal model is discussed in Section 4. The numerical comparison also draws our attention to the differences between various implementations of the coupling ray theory, based on various quasi–isotropic approximations (*Bulant and Klimeš, 2004*; *Klimeš and Bulant, 2004*).

In additional numerical tests summarized in Section 5, the exact analytical solution and the approximate analytical ray–theory solutions are compared with analogous numerical results of the general–purpose computer codes developed by the authors of the paper. These comparisons are very important in checking the equations, in debugging the 3-D ray tracing and coupling–ray–theory programs, in debugging single–purpose programs for the analytical solutions, and in testing the numerical accuracy of various computer codes. The exact analytical solution is numerically compared with the results of finite differences (*Vavryčuk, 1999*). The analytical solution of the equations of the coupling ray theory is compared with the results of the 3-D ray tracing packages ANRAY (*Pšenčík, 1998a,b*) and CRT (*Červený, Klimeš and Pšenčík, 1988*). The analytical solution of the equations of the coupling ray theory with the quasi–isotropic perturbation of travel times is compared with the results of the 3-D ray tracing package ANRAY. The analytical solution of the equations of the isotropic ray theory is compared with the results of the 3-D ray tracing package CRT.

2. MODEL FOR NUMERICAL COMPARISON

In the 1-D anisotropic *simplified twisted crystal* model, with density–normalized elastic moduli $a_{ijkl} = a_{ijkl}(x_3)$ and constant density ϱ, we take

$$a_{33K3} = 0 \quad . \tag{1}$$

The lower–case subscripts take values $i, j, k, ... = 1, 2, 3$, the upper–case subscripts take values $I, J, K, ... = 1, 2$. For plane wave $u_i = u_i(x_3)$ propagating along the x_3 axis, components u_K are fully separated from u_3. We choose elastic moduli a_{I3K3} in the form of

$$\begin{pmatrix} a_{1313} & a_{1323} \\ a_{2313} & a_{2323} \end{pmatrix} = v_0^2 \mathbf{B} \tag{2}$$

with

$$\mathbf{B} = \begin{pmatrix} 1 + \varepsilon\cos(2Kx_3) & \varepsilon\sin(2Kx_3) \\ \varepsilon\sin(2Kx_3) & 1 - \varepsilon\cos(2Kx_3) \end{pmatrix} \quad . \tag{3}$$

Refer to *Klimeš (2004)* for more details.

We use the simplified twisted crystal model designed by *Vavryčuk (1999)*. Parameter ε in (3), describing the degree of anisotropy, is

$$\varepsilon = \frac{-\gamma \sin^2(\theta)}{1+\gamma \sin^2(\theta)} \tag{4}$$

in the *Vavryčuk's (1999)* notation. The selected numerical values are

$$\gamma \sin^2(\theta) = 0.15 \times 0.75 = 0.1125 \quad . \tag{5}$$

The arithmetic average v_0^2 of density–normalized elastic moduli a_{1313} and a_{2323} is

$$v_0^2 = a_{44}[1+\gamma \sin^2(\theta)] \tag{6}$$

in the *Vavryčuk's (1999)* notation. The selected numerical values are

$$v_0^2 = 6.0\,\mathrm{km^2s^{-2}} \times [1+0.15 \times 0.75] = 6.675\,\mathrm{km^2s^{-2}} \quad . \tag{7}$$

The square of the reference isotropic velocity used in the quasi–isotropic perturbation of travel times is

$$v_R^2 = 6.9\,\mathrm{km^2s^{-2}} \quad . \tag{8}$$

Parameter K describing the rotation of the crystal axes about the x_3 axis has the value

$$K = 0.032\,\mathrm{km^{-1}} \quad . \tag{9}$$

The source–receiver distance corresponds to the crystal axes rotated through angle $\varphi = \pi$ radians,

$$x_3 = \frac{\pi}{K} \approx 98.17477 \quad . \tag{10}$$

Note that *Vavryčuk (1999)* also used $\frac{1}{6}$, $\frac{2}{6}$ and $\frac{3}{6}$ of the above value.

The *central resonant frequency* (*Klimeš, 2004*, sec. 3.4; *Lakhtakia and Meredith, 1999,* sec. 3) is

$$F = \left| \frac{v_0 K}{2\pi} \right| \approx 0.0132\,\mathrm{Hz} \tag{11}$$

and the *coupling frequency* (*Klimeš, 2004,* sec. 4.2) is

$$\left| \frac{2}{\varepsilon} \right| F \approx 0.260\,\mathrm{Hz} \quad . \tag{12}$$

The anisotropic–ray–theory travel times are

$$\tau_1 \approx 36.212310\,\mathrm{s} \quad , \qquad \tau_2 \approx 40.079682\,\mathrm{s} \quad . \tag{13}$$

Their arithmetic average, which is the best isotropic travel time, is

$$\tau \approx 38.145996\,\mathrm{s} \quad . \tag{14}$$

3. RELATIVE DIFFERENCES OF THE ONE–WAY PROPAGATOR MATRICES

For numerical comparison, we define the relative (with respect to the initial conditions) difference between one–way propagator matrices $\mathbf{U}$ and $\mathbf{U}_0$ as

$$\Delta = \sqrt{\tfrac{1}{2}\mathrm{Tr}\left([\mathbf{U}_0 - \mathbf{U}]^{\dagger}[\mathbf{U}_0 - \mathbf{U}]\right)} \quad . \tag{15}$$

This definition is equivalent to equation (87) of *Klimeš (2004)*, except for the resonant frequencies $f \in (F\sqrt{1-|\varepsilon|}, F\sqrt{1+|\varepsilon|})$, but numerically no visible difference between the definitions has been observed even at resonant frequencies.

If only the first columns $\mathbf{u}$ and $\mathbf{u}_0$ of propagator matrices $\mathbf{U}$ and $\mathbf{U}_0$ are available for comparison (package ANRAY), we define the relative difference analogously as

$$\Delta = \sqrt{[\mathbf{u}_0 - \mathbf{u}]^{\dagger}[\mathbf{u}_0 - \mathbf{u}]} \quad . \tag{16}$$

4. NUMERICAL COMPARISON OF RAY METHODS WITH THE EXACT SOLUTION THROUGH THE ANALYTICAL SOLUTIONS

The numerical comparison consists of two steps:
(A) The comparison of the numerically evaluated analytical solutions with the corresponding results of computer programs (finite differences, 3-D ray tracing packages ANRAY and CRT) in order to check the equations and to debug both the 3-D codes and single–purpose programs for the analytical solutions. For the summary of these test calculations, refer to Section 5.
(B) The comparison of the exact solution with the analytical solutions of the equations for the zero–order isotropic and anisotropic ray theories, for the coupling ray theory of *Coates and Chapman (1990)*, and for the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation of the coupling ray theory according to *Pšenčík (1998a)* and *Pšenčík and Dellinger (2001)*. The results of this comparison are demonstrated in this section.

4.1. Comparison of four analytical ray–theory solutions with the exact solution in the frequency domain

The relative differences of the analytical solutions of the equations for the zero–order isotropic and anisotropic ray theories, for the coupling ray theory of *Coates and Chapman (1990)*, and for the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation of the coupling ray theory according to *Pšenčík (1998a)* and *Pšenčík and Dellinger (2001)* from the exact solution are plotted on a log–log scale in Figure 1. The time–harmonic solutions are compared in the frequency interval $\langle 0.001\,\mathrm{Hz}, 10\,\mathrm{Hz}\rangle$, with frequency step $\Delta f = 0.00025\,\mathrm{Hz}$ in the subinterval $\langle 0.001\,\mathrm{Hz}, 0.1\,\mathrm{Hz}\rangle$, step $\Delta f = 0.0025\,\mathrm{Hz}$ in the subinterval $\langle 0.1\,\mathrm{Hz}, 1\,\mathrm{Hz}\rangle$ and step $\Delta f = 0.025\,\mathrm{Hz}$ in the subinterval $\langle 1\,\mathrm{Hz}, 10\,\mathrm{Hz}\rangle$.

Note that the isotropic ray theory is applied to the isotropic model with the best propagation velocity as suggested by *Klimeš (2004)* and that the results of the quasi–isotropic perturbation of travel times depend on the reference velocity.

The differences from the exact solution correspond to the theoretical discussion of *Klimeš (2004)*. Neither the isotropic ray theory, nor the anisotropic ray theory is applicable at the coupling frequency. In the simplified twisted crystal model, in which the difference between the S–wave eigenvalues of the Christoffel matrix is constant along a ray, the high–frequency asymptotic error of the anisotropic ray theory is inversely proportional to frequency, as expected. On the other hand, *Thomson et al. (1992)* demonstrated analytically that the high–frequency asymptotic error of the anisotropic ray theory is inversely proportional to the second or higher root of frequency if the ray passes through the point of equal S–wave eigenvalues of the Christoffel matrix. Their analytical estimate can also be obtained as a high–frequency approximation to the solution of the coupling equation by *Coates and Chapman (1990,* eq. 30*; Bulant and Klimeš, 2002,* eq. 4*)* in the vicinity of the point of equal S–wave eigenvalues of the Christoffel matrix.

The coupling ray theory of *Coates and Chapman (1990)* yields excellent results in this model, except for the resonant frequencies, which are far outside the validity regions of the ray theories. The high–frequency asymptotic error of the coupling ray theory is inversely proportional to frequency, but is considerably smaller than the high–frequency asymptotic error of the anisotropic ray theory, by factor $\left|\frac{2}{\varepsilon}\right|\sqrt{1+\left(\frac{Kx_3}{2}\right)^2} \approx 36.8$ (*Klimeš, 2004*).

On the other hand, the coupling ray theory with the quasi–isotropic perturbation of travel times does not bridge the gap between the isotropic and anisotropic ray theories; there are frequencies where both the quasi–isotropic perturbation of travel times and the anisotropic ray theory display a relative error of 60%. Note that the only effect of the quasi–isotropic perturbation of travel times on the coupling ray theory is the calculation of the anisotropic–ray–theory travel times used in the coupling equation. Without the quasi–isotropic perturbation of travel times, the anisotropic–ray–theory travel times are calculated by the numerical quadratures of the corresponding slownesses along the reference ray (*Bulant and Klimeš, 2002,* eq. 2). With the quasi–isotropic perturbation of travel times, the anisotropic–ray–theory travel times are calculated from the reference travel time by the linear perturbation with respect to the density–normalized elastic moduli.

The quasi–isotropic projection of the Green tensor, the quasi–isotropic approximation of the Christoffel matrix, and the common ray approximations do not affect the coupling–ray–theory solution in the simplified twisted crystal model. The quasi–isotropic projection of the Green tensor and the quasi–isotropic approximation of the Christoffel matrix are demonstrated by *Bulant and Klimeš (2004)* in the "oblique twisted crystal model". The errors of the isotropic common ray approximation and anisotropic common ray approximation (*Bakker, 2002*) for both S–wave polarizations have been studied by *Klimeš and Bulant (2004)*.

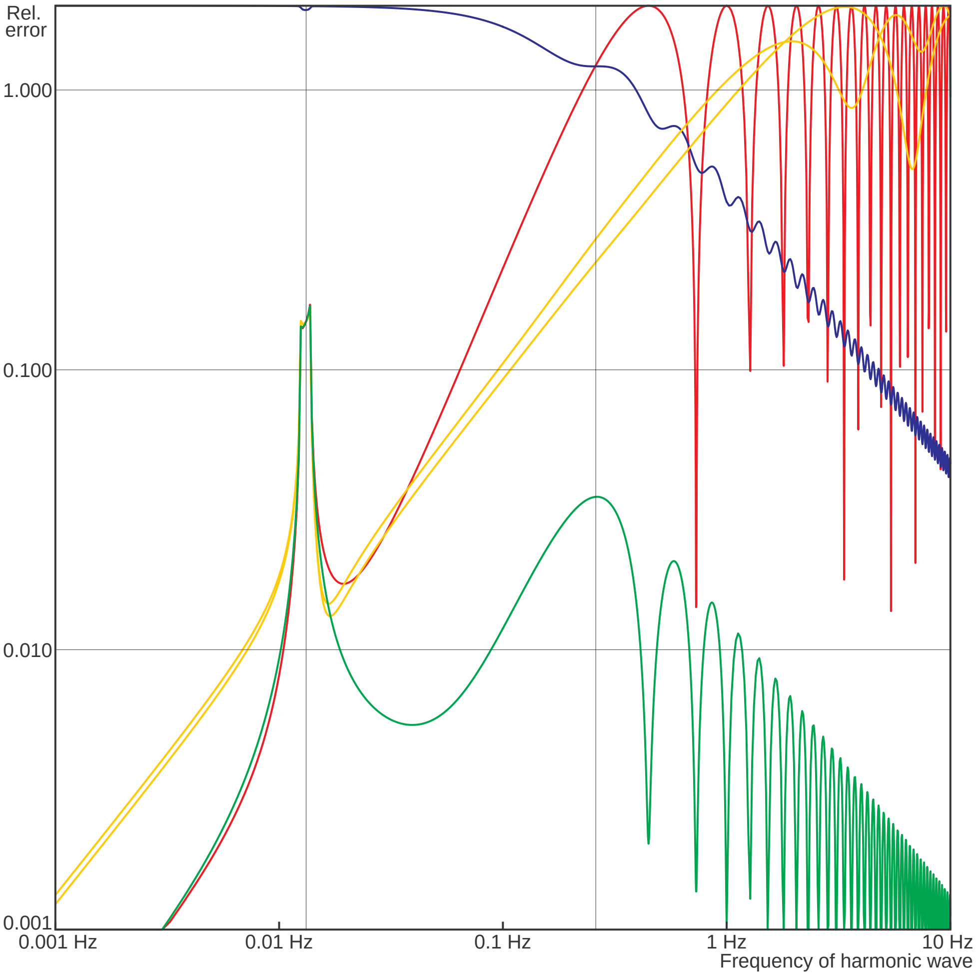

Fig. 1. The relative differences of the coupling ray theory of *Coates and Chapman (1990)* [green], the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation of the coupling ray theory according to *Pšenčík (1998a)* and *Pšenčík and Dellinger (2001)* [yellow], the zero–order anisotropic ray theory [blue] and the zero–order isotropic ray theory [red] from the exact solution. The two vertical lines denote the central resonant and coupling frequencies (11), (12). A relative error of 200% occurs, e.g., for opposite polarization, or opposite phase. The upper (up to 1 Hz) quasi–isotropic curve corresponds to reference velocity (8) used in package ANRAY, the lower quasi–isotropic curve corresponds to reference velocity (7).

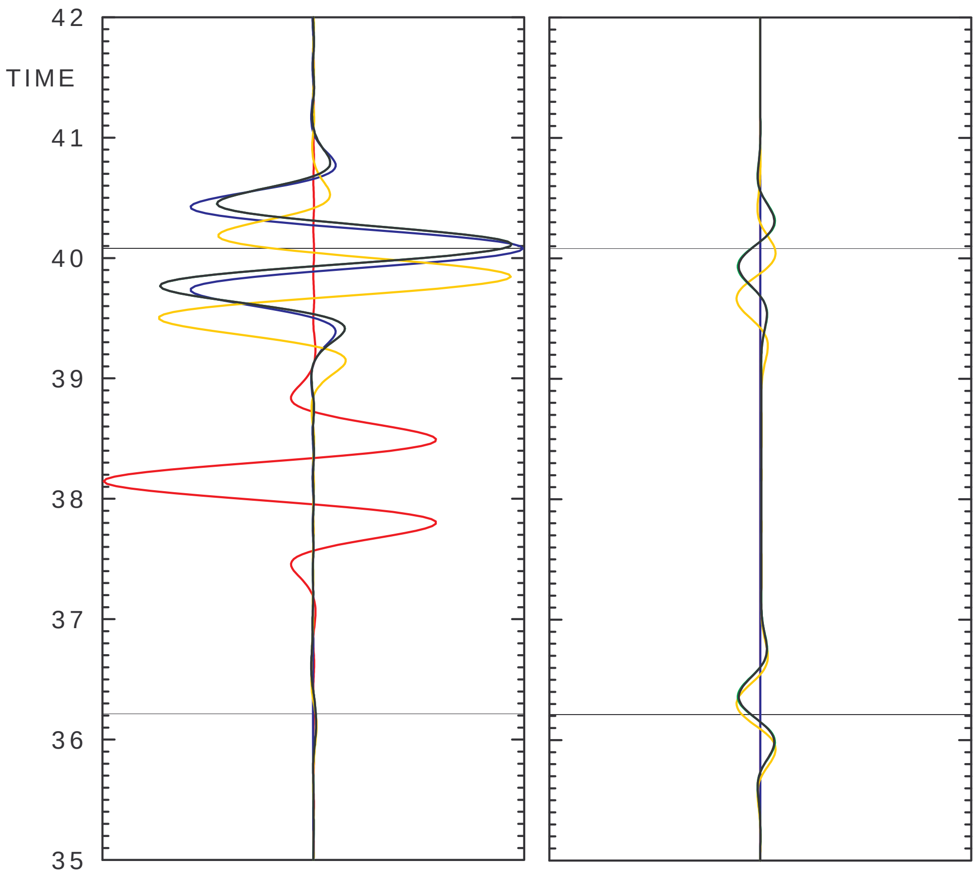

Fig. 2. Synthetic seismograms for the initial displacement in the x_1 direction modulated by the Gabor signal of prevailing frequency 1.3 Hz. The x_1 displacement is on the left, the x_2 displacement on the right. The exact solution is **black**, the coupling ray theory of *Coates and Chapman (1990)* is green and is obscured by the exact solution, the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation according to *Pšenčík (1998a)* and *Pšenčík and Dellinger (2001)* with reference velocity (8) is yellow, the zero–order anisotropic ray theory is blue, the zero–order isotropic ray theory is red and is obscured by the blue on the right. The two horizontal lines denote the anisotropic–ray–theory travel times (13).

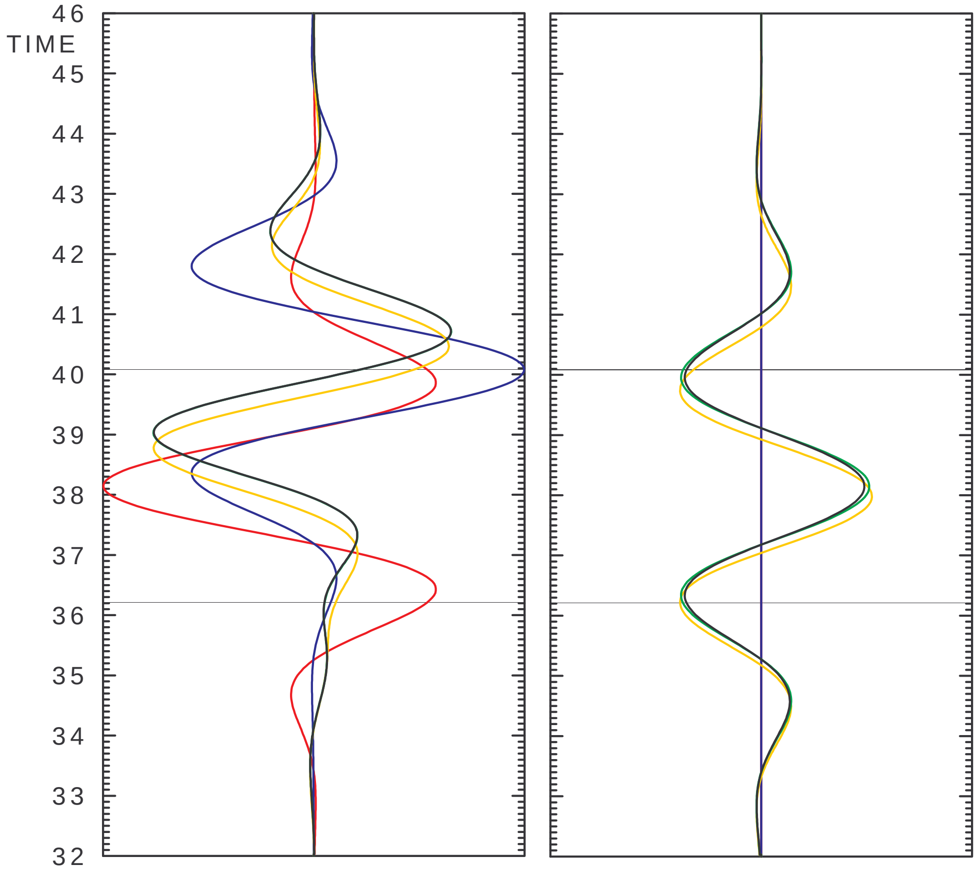

Fig. 3. Synthetic seismograms for the initial displacement in the x_1 direction modulated by the Gabor signal of prevailing frequency equal to coupling frequency 0.26 Hz. The x_1 displacement is on the left, the x_2 displacement on the right. The exact solution is **black**, the coupling ray theory of *Coates and Chapman (1990)* is green and is partly obscured by the black exact solution, the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation of the coupling ray theory according to *Pšenčík (1998a)* and *Pšenčík and Dellinger (2001)* with reference velocity (8) is yellow, the zero–order anisotropic ray theory is blue, the zero–order isotropic ray theory is red and is obscured by the blue on the right. The two horizontal lines denote the anisotropic–ray–theory travel times (13).

4.2. Synthetic seismograms for five analytical solutions

The synthetic seismograms corresponding to the exact solution and to the analytical solutions of the equations of the coupling ray theory of *Coates and Chapman (1990)*, for the quasi–isotropic perturbation of travel times included in the quasi–isotropic approximation of the coupling ray theory according to *Pšenčík (1998a)* and for the zero–order isotropic and anisotropic ray theories are shown in Figures 2 and 3. The reference velocity given by (8) is used.

The initial displacement at $x_3 = 0$ runs in the direction of the x_1 axis. Its time dependence has the form of the symmetric Gabor signal

$$\exp\left(-\left[\frac{2\pi f_0 t}{4}\right]^2\right)\cos\left(2\pi f_0 t\right) \tag{17}$$

with prevailing frequency

$$f_0 = 1.3\,\mathrm{Hz} \tag{18}$$

for Figure 2, filtered by the cosine band–pass filter described by frequencies

$$0.00\,\mathrm{Hz} \quad , \qquad 0.13\,\mathrm{Hz} \quad , \qquad 2.47\,\mathrm{Hz} \quad , \qquad 2.60\,\mathrm{Hz} \quad . \tag{19}$$

The frequency step for the fast Fourier transform is $\Delta f = 0.0125\,\mathrm{Hz}$. As the prevailing frequency in Figure 2 is five times larger than the coupling frequency, the two S–wave arrivals are clearly split, and the only visible difference between the exact solution and the anisotropic ray theory is the slightly different polarization. The coupling ray theory is nearly exact.

Analogous seismograms for the prevailing frequency, equal to the coupling frequency

$$f_0 = 0.26\,\mathrm{Hz} \quad , \tag{20}$$

are shown in Figure 3. The cosine band–pass filter is changed to

$$0.00\,\mathrm{Hz} \quad , \qquad 0.026\,\mathrm{Hz} \quad , \qquad 2.47\,\mathrm{Hz} \quad , \qquad 2.60\,\mathrm{Hz} \quad . \tag{21}$$

The frequency step for the fast Fourier transform is again $\Delta f = 0.0125\,\mathrm{Hz}$. The time shift due to the quasi–isotropic perturbation of travel times (*Klimeš, 2004,* sec. 4.3) can clearly be seen in both Figures 2 and 3. Since reference velocity v_R is greater than velocity v_0, the time shift increases from anisotropic travel time τ_1 to τ_2. For $v_R = v_0$, the quasi–isotropic seismogram would be shifted but not shrunk.

5. NUMERICAL COMPARISON OF ANALYTICAL SOLUTIONS WITH THE CORRESPONDING RESULTS OF COMPUTER PROGRAMS

The exact analytical solution is numerically compared with the results of finite differences (*Vavryčuk, 1999*). The analytical solution of the equations of the coupling ray theory is compared with the results of the 3-D ray tracing packages ANRAY (*Pšenčík, 1998a,b*) and CRT (*Červený et al., 1988*). The analytical solution of the equations of the coupling ray theory with the quasi–isotropic perturbation of travel times is compared with the results of the 3-D ray tracing package ANRAY. The analytical solution of the equations of the isotropic ray theory is compared with the results of the 3-D ray tracing package CRT.

These comparisons are very important in checking the equations, in debugging the 3-D ray tracing and coupling–ray–theory programs, in debugging the single–purpose programs for the analytical solutions, and in testing the numerical accuracy of various computer codes.

We have used the frequency interval $\langle 0.001\,\mathrm{Hz}, 1\,\mathrm{Hz}\rangle$, with frequency step $\Delta f = 0.00025\,\mathrm{Hz}$ in the subinterval $\langle 0.001\,\mathrm{Hz}, 0.1\,\mathrm{Hz}\rangle$ and step $\Delta f = 0.0025\,\mathrm{Hz}$ in the subinterval $\langle 0.1\,\mathrm{Hz}, 1\,\mathrm{Hz}\rangle$, for the comparison with finite differences. We have used the frequency interval $\langle 0.0\,\mathrm{Hz}, 2.6\,\mathrm{Hz}\rangle$ with frequency step $\Delta f = 0.0125\,\mathrm{Hz}$ for the comparison with the results of the 3-D ray tracing packages ANRAY and CRT.

5.1. Finite differences, exact solution

The time–harmonic finite–difference solution of the elastodynamic equation in the simplified twisted crystal model (*Vavryčuk, 1999*), calculated for the "unit" initial conditions in terms of displacement and stress, has been transformed to the initial conditions corresponding to the exact analytical solution for the one–way propagator matrix (*Klimeš, 2004*). The finite–difference solution, calculated in double precision, was then compared with the exact analytical solution, evaluated in single precision. The relative difference of the one–way propagator matrices is proportional to frequency and corresponds to the relative root–mean–square travel–time error of 0.000 000 4, which may correspond to the round–off errors in evaluating the exact analytical solution.

5.2. CRT package, isotropic and coupling ray methods

The numerically evaluated analytical solutions of the coupling–ray–theory equations and of the isotropic–ray–theory equations have been compared with the results of the CRT package. The relative differences between the numerical results of the CRT package (*Bucha and Klimeš, 1999*) and the corresponding analytical solutions are at the level corresponding to the round–off errors of the travel time, i.e. less than 0.1%. Note that the phase term $2\pi f\tau$ corresponding to travel time τ comes up to the order of 10^3. Since the absolute error of the phase term is reflected in the relative error in the one–way propagator matrix, relative differences of less than 0.001 correspond to relative travel–time errors of less than 0.000 001.

5.3. ANRAY package, coupling and quasi–isotropic ray methods

The ANRAY package is designed for the coupling ray theory with the isotropic common ray approximation, the quasi–isotropic approximation of the Christoffel matrix, and the quasi–isotropic perturbation of travel times (*Pšenčík, 1998a*; *Pšenčík and Dellinger, 2001*). Of these quasi–isotropic approximations, only the quasi–isotropic perturbation of travel times affects the coupling–ray–theory solution in the simplified twisted crystal model. The ANRAY package (*Pšenčík, 1998b*) enables the quasi–isotropic perturbation of travel times to be switched off optionally. The numerically evaluated analytical solutions of the coupling ray theory with and without the quasi–isotropic perturbation of travel times have been compared with the analogous results of the ANRAY package.

The coupling equation in the ANRAY package is solved numerically by the Euler method. The relative error of the one–way propagator matrix at frequency f due to the Euler method with integration step $\Delta\tau$ is

$$\Delta_{\text{Euler}} \approx \frac{1}{2}\frac{|\tau_2-\tau_1|}{2\tau}\,2\pi f\,\Delta\tau \quad , \tag{22}$$

see travel times (13) and (14). The relative error of the one–way propagator matrix due to the accumulation of the travel–time rounding errors is roughly

$$\Delta_{\text{round}} \approx \frac{1}{2}\frac{\tau}{\Delta\tau}\,2\pi f\,\tau\,\delta \quad , \tag{23}$$

where δ is the relative rounding error, roughly $\delta = 2^{-24}$ on a PC. The optimum step along the ray is then

$$\Delta\tau = \tau\sqrt{\frac{2\tau}{|\tau_2-\tau_1|}\,\delta} \quad . \tag{24}$$

The relative differences between the numerical results of package ANRAY at frequency $f = 2.6\,\text{Hz}$ and the corresponding analytical solutions are about 2% for the coupling ray theory with the quasi–isotropic perturbation of travel times, and about 2.5% without the quasi–isotropic perturbation of travel times. These numerical errors are in good agreement with estimate (23) indicating 2.8% for the relative error of the Euler method with $\delta = 2^{-24}$ and step $\Delta\tau = 0.025\,\text{s}$ along the ray, used to solve the coupling equation in the ANRAY package numerically. The accuracy of 0.1% of the CRT package (Section 5.2) has been achieved by numerical integration of the coupling equation using the method proposed by *Červený (2001)* and *Bulant and Klimeš (2002)*. Note that the numerical integration of the coupling equation by *Rümpker and Silver (2002,* eq. 6*)* based on the “forward propagator method” is a rough approximation to the more accurate method by *Červený (2001)* and *Bulant and Klimeš (2002)* based on the method of mean coefficients.

6. CONCLUSIONS

We have compared the exact analytical solution of the elastodynamic equation in the simplified twisted crystal model with the analytical solutions of the equations of the four ray methods, see Figure 1. The ray methods are (a) the coupling ray theory, (b) the coupling ray theory with the quasi–isotropic perturbation of travel times, (c) the anisotropic ray theory, (d) the isotropic ray theory. In the simplified twisted crystal model, the coupling ray theory is considerably more accurate than the isotropic and anisotropic ray theories. The error of the anisotropic ray theory is considerably larger than the error of the coupling ray theory at all high frequencies. In the simplified twisted crystal model, the quasi–isotropic perturbation of travel times makes the accuracy of the coupling ray theory considerably worse at frequencies higher than the coupling frequency. The quasi–isotropic perturbation of travel times thus should be avoided.

The exact analytical solution of the elastodynamic equation has been checked by comparison with *Vavryčuk*'s *(1999)* finite–difference code.

For additional information, including electronic reprints, computer codes and data, refer to the consortium research project "Seismic Waves in Complex 3-D Structures" ("http://sw3d.mff.cuni.cz").

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