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Simulating propagation of decoupled elastic waves using low-rank approximate mixed-domain integral operators for anisotropic media

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ABSTRACT
In elastic imaging, the extrapolated vector fields are decoupled into pure wave modes, such that the imaging condition produces interpretable images. Conventionally, mode decoupling in anisotropic media is costly as the operators involved are dependent on the velocity, and thus are not stationary. We develop an efficient pseudo-spectral approach to directly extrapolate the decoupled elastic waves using low-rank approximate mixed-domain integral operators on the basis of the elastic displacement wave equation. We apply \( k \)-space adjustment to the pseudo-spectral solution to allow for a relatively large extrapolation time-step. The low-rank approximation is, thus, applied to the spectral operators that simultaneously extrapolate and decompose the elastic wavefields. Synthetic examples on transversely isotropic and orthorhombic models show that, our approach has the potential to efficiently and accurately simulate the propagations of the decoupled quasi-P and quasi-S modes as well as the total wavefields, for elastic wave modeling, imaging and inversion.

INTRODUCTION
Multicomponent seismic data are increasingly acquired on land and at the ocean bottom in an attempt to better understand the geological structure and characterize oil and gas reservoirs. Seismic modeling, reverse-time migration (RTM), and full-waveform inversion (FWI) in areas with complex geology all require high-accuracy numerical algorithms for time extrapolation of waves. Because seismic waves propagate through the earth as a superposition of P- and S-wave modes, an elastic wave equation is usually more accurate for wavefield extrapolation than an acoustic wave equation. Wave mode decoupling can not only help elastic imaging to produce physically interpretable images, which characterize reflectivities of various reflection types (Wapenaar et al., 1987; Dellinger and Etgen, 1990; Yan and Sava, 2008), but also provide more opportunity to mitigate the parameter trade-offs in elastic waveform inversion (Wang and Cheng, 2015).

For isotropic media, far-field P and S waves can be separated by taking the divergence and curl in the extrapolated elastic wavefields (Aki and Richards, 1980; Sun...
and McMechan (2001). Alternatively, Ma and Zhu (2003) and Zhang et al. (2007) extrapolated vector P and S modes separately in an elastic wavefield by decomposing the wave equation into P- and S-wave components. In the meantime, decoupling of wave modes yields familiar scalar wave equations for P and S modes (Aki and Richards, 1980). In anisotropic media, one cannot, so simply, derive explicit single-mode time-space-domain differential wave equations. Generally, P and S modes do not respectively polarize parallel and perpendicular to the wave vectors, and thus are called quasi-P (qP) and quasi-S (qS) waves. They cannot be fully decoupled with divergence and curl operations (Dellinger and Etgen, 1990).

Anisotropic wave propagation can be formally decoupled in the wavenumber-domain to yield single-mode pseudo-differential equations (Liu et al., 2009). Unfortunately, these equations in time-space domain cannot be solved with traditional numerical schemes unless further approximation to the dispersion relation or phase velocity is applied (Etgen and Brandsberg-Dahl, 2009; Chu et al., 2011; Fowler and King, 2011; Zhan et al., 2012; Song and Alkhalifah, 2013; Wu and Alkhalifah, 2014; Du et al., 2014). To avoid solving the pseudo-differential equation, Xu and Zhou (2014) proposed a nonlinear wave equation for pseudoacoustic qP-wave with an auxiliary scalar operator depending on the material parameters and the phase direction of the propagation at each spatial location. All these efforts are restricted to pure-mode scalar waves and do not honor the elastic effects such as mode conversion. Cheng and Kang (2014) and Kang and Cheng (2012) have proposed approaches to propagate the partially decoupled wave modes using the so-called pseudo-pure-mode wave equations, and then obtain completely decoupled qP or qS waves by correcting the polarization deviation of the pseudo-pure-mode wavefields. Their approaches honor the kinematics of all wave modes but may distort the reflection/transmission coefficients if high contrasts exist in the velocity fields.

Alternatively, many have developed approaches to decouple qP- and qS-wave modes from the extrapolated elastic wavefields. Dellinger and Etgen (1990) generalized the divergence and curl operations to anisotropic media by constructing separators as polarization projection in the wavenumber-domain. To tackle heterogeneity, these mode separators were rewritten by Yan and Sava (2009) as nonstationary spatial filters determined by the local polarization directions. Zhang and McMechan (2010) proposed a wavefield decomposition method to separate elastic wavefields into vector qP- and qS-wave fields for vertically transverse isotropic (VTI) media. Accordingly, Cheng and Fomel (2014) proposed fast mixed-domain algorithms for mode separation and vector decomposition in heterogeneous anisotropic media by applying low-rank approximation to the involved Fourier integral operators (FIos) of the general form.

The motivation of this study is to develop an efficient approach to propagate and decouple the elastic waves for general anisotropic media. The primary strategy is to merge the numerical solutions for time extrapolation and vector decomposition into a unified Fourier integral framework and speed up the solutions using the low-rank approximation. This paper is organized as follows. We first demonstrate a pseudo-spectral solution to extrapolate the elastic displacement wavefields in time-
domain. Then we propose to merge the spectral operations for time extrapolation into the integral framework for vector decomposition of the wave modes. Applying low-rank approximations to the involved mixed-domain matrices, we obtain an efficient algorithm for simultaneous propagating and decoupling the elastic wavefields. We demonstrate the validity of the proposed method using 2-D and 3-D synthetic examples on the transversely isotropic (TI) and orthorhombic models with increasing complexity.

PROPAGATING COUPLED ELASTIC WAVEFIELDS

Following Carcione (2007), we denote the spatial variables \( x, y \) and \( z \) of a right-hand Cartesian system by the indices \( i, j, \ldots = 1, 2 \) and 3, respectively, the position vector by \( \mathbf{x} \), a partial derivative with respect to a variable \( x_i \) with \( \partial_i \), and the first and second time derivatives with \( \partial_t \) and \( \partial_{tt} \). Matrix transposition is denoted by the superscript “\( T \)”. We also denote \( \sqrt{-1} \) by \( i \), the scalar and matrix products by the symbol “\( \cdot \)”, the dyadic product by the symbol “\( \otimes \)”. The Einstein convention of repeated indices is assumed unless otherwise specified.

Pseudo-spectral solution of the elastic wave equation

Wave propagation in general anisotropic elastic media is governed by the linearized momentum balance law and a linear constitutive relation between the stress and strain tensors. These governing equations can be combined to write the displacement formalism as,

\[
\rho \partial_{tt}^2 \mathbf{u} = \nabla \cdot \left[ \mathbf{C} \cdot (\nabla^T \cdot \mathbf{u}) \right] + \mathbf{f},
\]

with \( \mathbf{u} = (u_x, u_y, u_z)^T \) represents the vector wavefields, \( \mathbf{f} \) is the body force vector per unit volume, \( \mathbf{C} \) is the \( 6 \times 6 \) elasticity matrix representing the stiffness tensor with the Voigt’s menu, and the spatial differential operator \( \nabla \) has the following matrix representation:

\[
\nabla = \begin{pmatrix}
\partial_x & 0 & 0 & \partial_y & \partial_z \\
0 & \partial_y & 0 & \partial_z & 0 \\
0 & 0 & \partial_z & \partial_y & \partial_x
\end{pmatrix}.
\]

The pseudo-spectral method calculates the spatial derivatives using the fast Fourier transform (FFT), while approximating the temporal derivative with a finite-difference. Neglecting the source term, equation 2 is rewritten in the spatial Fourier-domain for a homogeneous medium as,

\[
\partial_{tt}^2 \mathbf{\hat{u}} + \mathbf{\Gamma} \mathbf{\hat{u}} = \mathbf{0},
\]

in which \( \mathbf{\hat{u}} \) is the wavefields in the wavenumber-domain, \( \mathbf{k} = (k_x, k_y, k_z) \) is the wavenumber vector, and \( \mathbf{\Gamma} = 1/\rho \mathbf{L} \cdot \mathbf{C} \cdot \mathbf{L}^T \) represents the \( 3 \times 3 \) density normalized Christoffel matrix with the wavenumber-domain counterpart of the space differential
operator (removing the imaginary unit \(i\)) satisfies,

\[
L = \begin{pmatrix}
    k_x & 0 & 0 & k_z & k_y \\
    0 & k_y & 0 & k_z & 0 \\
    0 & 0 & k_z & k_y & k_x
\end{pmatrix}.
\] (4)

To calculate the 2nd-order temporal derivatives, we use the standard leapfrog scheme, i.e.,

\[
\partial_{tt} u_i^{(n)} = \frac{u_i^{(n+1)} - 2u_i^{(n)} + u_i^{(n-1)}}{\Delta t^2},
\] (5)

in which \(\Delta t = t^{n+1} - t^n\) is the time-step. For constant density homogeneous media, applying the two-step time-marching scheme leads to the pseudo-spectral formula:

\[
\partial_{tt} u^{(n)} = \Psi u^{(n)},
\] (6)

with the spectral operator defined with the following kernel:

\[
\Psi := (2\pi)^{-3} \int \int \Gamma(k)e^{ik \cdot (x-y)} dy dk.
\] (7)

Phase terms in the integral operator can be absorbed into forward and inverse Fourier transforms. This implies that the wavefields are first transformed into wavenumber-domain using forward FFTs, then multiplied with the corresponding components of the Christoffel matrix, and finally transformed back into space-domain using inverse FFTs. For locally smooth media, we use a spatially varying Christoffel matrix to tackle the heterogeneity, i.e.,

\[
\Psi := (2\pi)^{-3} \int \int \Gamma(x, k)e^{i k \cdot (x-y)} dy dk.
\] (8)

The extended formation of this pseudo-spectral elastic wave propagator is shown in Appendix B. Spectral methods are characterized by the use of Fourier basis functions to describe the field variables and have the advantages over finite-difference schemes that the mesh requirements are more relaxed (Kosloff et al., 1989; Liu and Li, 2000).

**Adjustment to the pseudo-spectral solution**

Generally, the two-step time-marching pseudo-spectral solution is limited to a small time-step, as larger time-steps lead to numerical dispersion and stability issues. At more computational costs, high-order finite-difference (Dablain, 1986) can be applied to address this difficulty. As an alternative to second-order temporal differencing, a time integration technique based on rapid expansion method (REM) can provide higher accuracy with less computational efforts (Kosloff et al., 1989). As Du et al. (2014) demonstrated, one-step time marching schemes (Zhang and Zhang, 2009; Sun and Fomel, 2013), especially using optimized polynomial expansion, usually give more
Propagate decoupled anisotropic elastic waves accurate approximations to heterogeneous extrapolators for larger time-steps. In this section, we discuss a strategy to extend the time-step for the previous two-step time-marching pseudo-spectral scheme according to the eigenvalue decomposition of the Christoffel matrix.

Since the Christoffel matrix is symmetric positive definite, it has a unique eigen-decomposition of the form:

\[ \Gamma = \sum_{i=1}^{3} \lambda_i^2 \mathbf{a}_i \otimes \mathbf{a}_i, \]  

(9)

where \( \lambda_i^2 \)'s are the eigenvalues and \( \mathbf{a}_i \)'s are the eigenvectors of \( \Gamma \), with \( \mathbf{a}_i \cdot \mathbf{a}_j = \delta_{ij} \). The three eigenvalues correspond to phase velocities of the three wave modes with \( \lambda_i = v_i k \) (in which \( k = |\mathbf{k}| \), and \( v_i \) represents the phase velocity) representing the circular frequency, and the corresponding eigenvector \( \mathbf{a}_i = (a_{ix}, a_{iy}, a_{iz}) \) represents the normalized polarization vector for the given mode. An alternative form of the above decomposition yields:

\[ \Gamma = \mathbf{Q} \Lambda \mathbf{Q}^T, \]  

(10)

with

\[ \Lambda = \begin{pmatrix} \lambda_1^2 & 0 & 0 \\ 0 & \lambda_2^2 & 0 \\ 0 & 0 & \lambda_3^2 \end{pmatrix}, \]  

(11)

\[ \mathbf{Q} = \begin{pmatrix} a_{1x} & a_{2x} & a_{3x} \\ a_{1y} & a_{2y} & a_{3y} \\ a_{1z} & a_{2z} & a_{3z} \end{pmatrix}. \]  

(12)

Note \( \mathbf{Q} \) is an orthogonal matrix, i.e., \( \mathbf{Q}^{-1} = \mathbf{Q}^T \).

The eigenvalues represent the frequencies and satisfy the condition given by,

\[ \lambda_i = v_i k \leq 2\pi f_{\text{max}}, \]  

(13)

in which \( f_{\text{max}} \) is the maximum frequency of the source. Therefore, we suggest to filter out the high-wavenumber components in the wavefields beyond \( 2\pi f_{\text{max}} / v_{\text{min}} \) (\( v_{\text{min}} \) is the minimum phase velocity in the computational model) caused by the numerical errors to enhance numerical stability.

According to above eigen-decomposition, we apply the \( k \)-space adjustment to our pseudo-spectral scheme by modifying the eigenvalues of Christoffel matrix for the anisotropic elastic wave equation (see Appendix C), i.e.,

\[ \tilde{\Lambda} = \begin{pmatrix} \lambda_1^2 sinc^2(\lambda_1 \Delta t/2) & 0 & 0 \\ 0 & \lambda_2^2 sinc^2(\lambda_2 \Delta t/2) & 0 \\ 0 & 0 & \lambda_3^2 sinc^2(\lambda_3 \Delta t/2) \end{pmatrix}. \]  

(14)

Thus this adjustment inserts a modified Christoffel matrix, i.e., \( \Gamma = \mathbf{Q} \tilde{\Lambda} \mathbf{Q}^T \), into the original pseudo-spectral formula on the basis of equations 6 and 8. Note that the \( k \)-space adjustment to the pseudo-spectral solution has been widely used in acoustic and ultrasound \([\text{Bojarski}, 1982] [\text{Tabei et al., 2002}] \) and elastic isotropic wavefield simulation \([\text{Liu}, 1995] [\text{Firouzi et al., 2012}] \).
PROPAGATING DECOUPLED ELASTIC WAVEFIELDS

Above pseudo-spectral operators propagate the elastic wavefields as a superposition of qP- and qS-wave modes. To obtain physically interpretable results for seismic imaging and waveform inversion, wave mode decoupling is required during wavefield extrapolation. The key concept of mode decoupling is based on polarization. In a general anisotropic medium, the qP and qS modes do not polarize parallel and perpendicular to the wave vectors. Moreover, unlike the well-behaved qP mode, the two qS modes do not consistently polarize as a function of the propagation direction (or wavenumber) and thus cannot be designated as SV and SH waves, except in isotropic and TI media (Winterstein, 1990; Crampin, 1991). Even for a TI medium, it is a challenge to find the right solution of the shear singularity problem and obtain two completely separated S-modes with correct amplitudes (Yan and Sava, 2011; Cheng and Fomel, 2014). Therefore, we restrict to extrapolate the decoupled qP- and qS-wave modes in this paper.

Vector decomposition of the elastic wave modes

According to Zhang and McMechan (2010), one can decompose qP and qS modes in the elastic wavefields for a homogeneous anisotropic medium using:

$$u_i^{(m)}(k) = d_{ij}^{(m)}(k)\tilde{u}_j(k),$$  \hspace{1cm} (15)

where \( m = \{qP, qS\} \), \( i, j = \{x, y, z\} \), and the decomposition operators satisfy:

$$d_x^{(qP)}(k) = a_x^2(k),$$
$$d_y^{(qP)}(k) = a_y^2(k),$$
$$d_z^{(qP)}(k) = a_z^2(k),$$
$$d_{xy}^{(qP)}(k) = a_x(k)a_y(k),$$
$$d_{xz}^{(qP)}(k) = a_x(k)a_z(k),$$
$$d_{yz}^{(qP)}(k) = a_y(k)a_z(k),$$

and

$$d_x^{(qS)}(k) = a_y^2(k) + a_z^2(k),$$
$$d_y^{(qS)}(k) = a_y^2(k) + a_z^2(k),$$
$$d_z^{(qS)}(k) = a_x^2(k) + a_z^2(k),$$
$$d_{xy}^{(qS)}(k) = -a_x(k)a_y(k),$$
$$d_{xz}^{(qS)}(k) = -a_x(k)a_z(k),$$
$$d_{yz}^{(qS)}(k) = -a_y(k)a_z(k),$$

in which \( a_x(k), a_y(k) \) and \( a_z(k) \) represent the \( x-, y- \) and \( z- \) components of the normalized polarization vector of qP-wave.

As demonstrated by Cheng and Fomel (2014), one can decompose the wave modes in a heterogeneous anisotropic medium using the following mixed-domain integral
Propagate decoupled anisotropic elastic waves

For heterogeneous anisotropic media, the wavefield propagator (equation 6) and the vector decomposition operators (equation 18) are both in the general form of FIOs. Naturally, we merge them to derive a new mixed-domain integral solution for extrapolating the decoupled elastic wavefields:

\[
\begin{align*}
    u_x^{(m)}(x, t + \Delta t) &= -u_x^{(m)}(x, t - \Delta t) + \int e^{ikx w_{xx}^{(m)}}(x, k) \tilde{u}_x(k, t) \, dk + \int e^{ikx w_{xy}^{(m)}}(x, k) \tilde{u}_y(k, t) \, dk + \int e^{ikx w_{xz}^{(m)}}(x, k) \tilde{u}_z(k, t) \, dk, \\
    u_y^{(m)}(x, t + \Delta t) &= -u_y^{(m)}(x, t - \Delta t) + \int e^{ikx w_{yx}^{(m)}}(x, k) \tilde{u}_x(k, t) \, dk + \int e^{ikx w_{yy}^{(m)}}(x, k) \tilde{u}_y(k, t) \, dk + \int e^{ikx w_{yz}^{(m)}}(x, k) \tilde{u}_z(k, t) \, dk, \\
    u_z^{(m)}(x, t + \Delta t) &= -u_z^{(m)}(x, t - \Delta t) + \int e^{ikx w_{zx}^{(m)}}(x, k) \tilde{u}_x(k, t) \, dk + \int e^{ikx w_{zy}^{(m)}}(x, k) \tilde{u}_y(k, t) \, dk + \int e^{ikx w_{zz}^{(m)}}(x, k) \tilde{u}_z(k, t) \, dk,
\end{align*}
\]  

(19)

with the propagation matrices for the decoupled wave modes given as

\[
\begin{align*}
    w_{ij}^{(m)}(x, k) &= d_{ki}^{(m)}(x, k) w_{kj}(x, k),
\end{align*}
\]  

(20)

in which \(w_{kj}(x, k)\) is defined by the spatially varying Christoffel matrix and the length of time-step, namely

\[
\begin{align*}
    w_{kk}(x, k) &= 2 - \Delta t^2 \Gamma_{kk}(x, k), \\
    w_{kj}(x, k) &= -\Delta t^2 \Gamma_{kj}(x, k).
\end{align*}
\]  

(21)

The extended formulation of equation (20) is given in Appendix B. Note the symmetry properties exist: \(d_{ki}^{(m)} = d_{ik}^{(m)}\) and \(w_{kj} = w_{jk}\), and the modified Christoffel matrix will be used if the \(k\)-space adjustment is applied for the pseudo-spectral solutions.

To drive the time extrapolation of the decomposed wavefields using equation (19) we must update the total elastic wavefields by superposing \(qP\)- and \(qS\)-waves at each time-step using

\[
\begin{align*}
    u_x(x) &= u_x^{(qP)}(x) + u_x^{(qS)}(x), \\
    u_y(x) &= u_y^{(qP)}(x) + u_y^{(qS)}(x), \\
    u_z(x) &= u_z^{(qP)}(x) + u_z^{(qS)}(x),
\end{align*}
\]  

(22)

Thus equations (19) to (22) compose the spectral-like operators to simultaneously extrapolate and decouple the elastic wavefields for 3D anisotropic media. The computation
complexity of the straightforward implementation of the integral operators in equations \[8\] and \[19\] is \(O(N_x^2)\), which is prohibitively expensive when the size of model \(N_x\) is large.

To tackle strong heterogeneity due to fast varying stiffness coefficients, we suggest to split the displacement equation into the displacement-stress equation and then solve it using the staggered-grid pseudo-spectral scheme (Ozdenvar and McMechan, 1996; Carcione, 1999; Bale, 2003). Note when using staggered grids, the operators to extrapolate the decoupled wave modes must be modified in order to account for the shifts in medium properties and fields variables. We will investigate this issue in the future work.

### FAST ALGORITHM USING LOW-RANK DECOMPOSITION

As proposed by Cheng and Fomel (2014), low-rank decomposition of the mixed-domain matrix \(d(x, k)\) in equation \[18\] yields very efficient algorithm for mode decoupling in heterogeneous anisotropic media. We find that the same strategy works for numerical implementations of above pseudo-spectral operators for elastic wave propagation.

For example, the mixed-domain matrix, i.e., \(w(x, k)\) or \(\tilde{w}(x, k)\) in the FIOs, can be approximated by the following separated representation (Fomel et al., 2013):

\[
W(x, k) \approx \sum_{m=1}^{M} \sum_{n=1}^{N} B(x, k_m) A_{mn} C(x_n, k),
\]

in which \(B(x, k_m)\) is a mixed-domain matrix with reduced wavenumber dimension \(M\), \(C(x_n, k)\) is a mixed-domain matrix with reduced spatial dimension \(N\), \(A_{mn}\) is a \(M \times N\) matrix with \(N\) and \(M\) representing the rank of this decomposition. Physically, a separable low-rank approximation amounts to selecting a set of \(N\) (\(N \ll N_x\)) representative spatial locations and \(M\) (\(M \ll N_x\)) representative wavenumbers. Construction of the separated representation follows the method of Engquist and Ying (2009). The ranks \(M\) and \(N\) are dependent on the complexities (heterogeneity and anisotropy) of the medium and the estimate of the approximation accuracy to the mixed-domain matrices (In the numerical examples, we aim for the relative single-precision accuracy of \(10^{-6}\)). More explanations on low-rank decomposition is available in Fomel et al. (2013) and Cheng and Fomel (2014). As we observe, the ranks are generally very small for our applications. For homogeneous media, the ranks naturally reduce to 1. If there is heterogeneity, the ranks increase to 2 for isotropic media but exceed 2 for anisotropic media. The \(k\)-space adjustment may slightly increase the ranks for the heterogeneous media.

Thus the above low-rank approximation speeds up computation of the FIOs since

\[
\int e^{ikx} W(x, k) \tilde{u}_j(k) \, dk \\
\approx \sum_{m=1}^{M} B(x, k_m) \left( \sum_{n=1}^{N} A_{mn} \left( \int e^{ikx} C(x_n, k) \tilde{u}_j(k) \, dk \right) \right).
\]

(24)
Evaluation of the last formula is effectively equivalent to applying \( N \) inverse FFTs each time-step. Accordingly, the computation complexity reduces to \( O(NN_x \log N_x) \). In multiple-core implementations, the matrix operations in equation 17 are easy to parallelize.

**EXAMPLES**

We will first demonstrate the proposed approach on two-layer TI and orthorhombic models, and then on the complex SEG Hess VTI and BP 2007 TTI models, respectively.

**2D two-layer VTI/TTI model**

The first example is on a 2D two-layer model, in which the first layer is a VTI medium with \( v_{p0} = 2500 \text{m/s}, v_{s0} = 1200 \text{m/s}, \epsilon = 0.2, \) and \( \delta = -0.2 \), and the second layer is a tilted TI (TTI) medium with \( v_{p0} = 3600 \text{m/s}, v_{s0} = 1800 \text{m/s}, \epsilon = 0.2, \delta = 0.1 \), and \( \theta = 30^\circ \). A point source is placed at the center of this model. Firstly, we compare the synthetic elastic wavefields by solving the elastic displacement wave equation using the 10th-order explicit finite-difference (FD) and low-rank pseudo-spectral schemes (with or without the \( k \)-space adjustment), respectively. Figure 1 shows the wavefield snapshots at the time of 0.3 s using the spatial sampling \( \Delta x = \Delta z = 5 \text{m} \) and time-step \( \Delta t = 0.5 \text{ms} \). Only the low-rank pseudo-spectral solutions with the \( k \)-space adjustment are displayed because the three schemes produce very similar results. The vertical slices through the z-components of the elastic wavefields show little differences among them (Figure 2). For the low-rank pseudo-spectral scheme, the ranks are all 2 for the decomposition of the mixed-domain matrices \( w_{xx}, w_{zz} \) and \( w_{xz} \) in equation 21, and the \( k \)-space adjustment doesn’t change the ranks. It takes CPU time of 0.20, 0.23 and 0.23 seconds for them to finish the wavefield extrapolation of one time-step. Additional 4.3 and 8.2 seconds have been used to finish the low-rank decomposition of the involved mixed-domain matrices before wavefield extrapolation. We observe the FD scheme unstable if the time-step is increased to 1.0 ms and the low-rank pseudo-spectral scheme unstable if the time-step is increased to 2.0 ms (with unchanged spatial sampling). However, the low-rank pseudo-spectral solution using the \( k \)-space adjustment produces acceptable results even the time-step is increased to 3.0 ms and the maximum time exceeds 3 s. Figure 3 and Figure 4 compare the wavefield snapshots and the vertical slices at the time of 0.6 s using the three schemes with the increased spatial sampling (namely \( \Delta x = \Delta z = 10 \text{m} \)). The FD scheme tends to exhibit dispersion artifacts with the chosen model size and extrapolation step, while low-rank pseudo-spectral scheme exhibit acceptable accuracy. The \( k \)-space adjustment permits larger time-steps without reducing accuracy or introducing instability. For this example, it has produced the best results with less numerical dispersion. Thanks to the larger spatial and temporal sampling, the same CPU time is used for each scheme as in Figure 1. In addition, only the ranks for the low-rank
decomposition of the matrix $w_{12}$ reduce to 1 when we change the tilt angle of the second layer to 0.

![Diagram](image)

Figure 1: Horizontal and vertical components of the elastic wavefields at the time of 0.3 s synthesized by solving the 2nd-order elastic wave equation with $\Delta x = \Delta z = 5$ m and $\Delta t = 0.5$ ms.

Secondly, we compare two approaches to get the decoupled elastic wavefields during time extrapolation. The first approach uses the low-rank pseudo-spectral algorithm to synthesize the elastic wavefields and then apply the low-rank vector decomposition algorithm (Cheng and Fomel, 2014) to get the vector $qP$- and $qSV$-wave fields (Figure 5). The second extrapolates the decoupled $qP$- and $qSV$-wave fields using the proposed low-rank mixed-domain integral operations (Figure 6). Extrapolation steps of $\Delta x = \Delta z = 10$ m and $\Delta t = 1.0$ ms are used in this example. The ranks are still 2 for the involved low-rank decomposition of the propagation matrices defined in equation 20. The two approaches produce comparable elastic wavefields, in which we can observe all transmitted and reflected waves including mode conversions. For one step of time extrapolation, it takes the CPU time of 0.6 ms for the first approach and 0.5 ms for the second. This means that merging time extrapolation and vector decomposition into a unified Fourier integral framework provides more efficient solution than operating them in sequence for anisotropic media thanks to the reduced number of forward and inverse FFTs.

**3D two-layer VTI/orthorhombic model**

Figure 7 shows synthetic vector displacement fields using the proposed approach for a 3-D two-layer model, with a horizontal reflector at 1.167 km. The first layer is a VTI medium with $v_{p0} = 2500m/s$, $v_{s0} = 1400m/s$, $\epsilon = 0.25$, $\delta = 0.05$, and $\gamma = 0.15$, and the second is an orthorhombic medium representing a vertically fractured TI formation (Schoenberg and Helbig, 1997; Tsvankin, 2001), which has the parameters $v_{p0} = 3000m/s$, $v_{s0} = 1600m/s$, $\epsilon_1 = 0.30$, $\epsilon_2 = 0.15$, $\delta_1 = 0.08$, $\delta_2 = -0.05$, $\delta_3 = -0.10$, $\gamma_1 = 0.20$ and $\gamma_2 = 0.05$. A exploration source is located at the center of the model. We achieve efficient simulation of dispersion-free 3D elastic wave propagation for the decoupled and total displacement fields. Shear wave splitting can be observed in the $qS$-wave fields.
Figure 2: Vertical slices through the vertical components of the synthetic elastic wavefields at $x = 0.75$ km: (a) 10th-order FD, (b) low-rank pseudo-spectral and (c) low-rank pseudo-spectral using the $k$-space adjustment.

Figure 3: Vertical components of the elastic wavefields at the time of 0.6 s synthesized using three schemes with the same spatial sampling $\Delta x = \Delta z = 10$ m: (a) 10th-order FD and (b) low-rank pseudo-spectral with $\Delta t = 1.5$ ms, and (c) low-rank pseudo-spectral solution using the $k$-space adjustment with $\Delta t = 3.0$ ms.
Figure 4: Vertical slices through the vertical components at \( x = 1.5 \) km in Figure 3: (a) 10th-order FD, (b) low-rank pseudo-spectral and (c) low-rank pseudo-spectral using the \( k \)-space adjustment.

Figure 5: Elastic wavefields at the time of 0.6 s synthesized by using low-rank pseudo-spectral solution of the displacement wave equation followed with low-rank vector decomposition: (a) \( x \)- and (b) \( z \)-components of the displacement wavefields; (c) \( x \)- and (d) \( z \)-components of the \( qP \)-wave fields; (e) \( x \)- and (f) \( z \)-components of the \( qSV \)-wave fields.
SEG Hess VTI model

Then we demonstrate the approach in the 2D Hess VTI model (Figure 8). Vertical qS-wave velocity is set to equal half the vertical qP-wave velocity everywhere. A point-source is placed at location of (13.264, 4.023) km. For comparison, spatial step length $\Delta x = \Delta z = 40.0$ ft and time-step $\Delta t = 1.0$ ms are used in this example. Figure 9 displays the decoupled and total displacement fields synthesized by using the low-rank pseudo-spectral algorithm that simultaneously extrapolate the decoupled qP- and qSV-wave modes. The ranks $N, M$ are in $[8, 10]$ for the low-rank decomposition of the involved matrices (The ranks reduce to $[1, 3]$ if we only propagate the coupled elastic wavefields). The wavefield snapshots show that the proposed wave propagator honors the elastic effects such as mode conversion. It takes the CPU time of 111.6 s to decompose the mixed-domain matrices in advance, and about 9397.7 s to extrapolate the decoupled wavefields to the maximum time of 1100.0 s. Figure 10 displays the total displacement fields synthesized by the 10th-order FD solution of the elastic wave equation and the decoupled qP- and qSV-wave fields using the low-rank vector decomposition for heterogeneous TI media (Cheng and Fomel, 2014). The ranks are in $[6, 7]$ for the decomposition of the involved mode decoupling matrices $d_{ij}$. The FD solution shows strong numerical dispersion of the qSV-waves due to inadequate sampling because the modeling of qSV-wave using FD scheme demands finer grid cell size. Except the CPU time of 36.7 s to decompose the mixed-domain matrices
Figure 7: Synthesized decomposed and total elastic wavefields for an orthorhombic model with a VTI overburden: qP (left), qS (mid) and total (right) elastic displacement fields (top: x-component, mid: y-component, bottom: z-component).
for mode decoupling, it takes 568.0 s to extrapolate and 4690.3 s to decouple the elastic wavefields to get qP- and qS-wave fields for all the time-steps. To achieve the same good quality as the low-rank pseudo-spectral solution in Figure 8, we decrease the spatial sampling to $\Delta x = \Delta z = 20.0$ ft and the temporal sampling to 0.5 ms. Except the CPU time of 133.8 s to decompose the mixed-domain matrices for mode decoupling, it takes 3922.8 s to extrapolate and 14212.0 s to decouple the elastic wavefields to the maximum time. This means the low-rank pseudo-spectral scheme more efficient to obtain decoupled elastic wavefields for TI media.

Figure 8: SEG/Hess VTI model with parameters of (a) vertical P-wave velocity, Thomsen coefficients (b) $\epsilon$ and (c) $\delta$.

BP 2007 TTI model

The last example displays the application to the BP 2007 TTI model (Figure 11). Vertical qS-wave velocity is set to equal sixty percent of the vertical qP-wave velocity everywhere. Extrapolation steps of $\Delta x = \Delta z = 12.5$ m and $\Delta t = 1.0$ ms are used here. Because the principal axes of the medium are not aligned with the Cartesian axes, we have apply the Bond transformation to get the stiffness matrix under the Cartesian system. Before wavefield extrapolation, separated representations of the mixed operator matrixes are constructed using the low-rank decomposition approach within the computational zone. For this complex model, the ranks are about 30 for the decomposition of the involved matrixes. As shown in Figure 12, the approach describes very well the propagations of the decoupled qP- and qS-waves as well as the total displacement fields even for this complex TTI model. We can clearly observe the converted waves from the dipping salt flanks and other strong-contrast interfaces. And the qP- and qS-waves are free of numerical dispersion in the decoupled and total wavefields.
Figure 9: Synthesized decoupled and total displacement fields using the low-rank pseudo-spectral solution with the $k$-space adjustment that simultaneously extrapolate and decouple qP- and qSV-wave fields in SEG/Hess VTI model: (a) x- and (b) z-components of qP-wave fields; (c) x- and (d) z-components of qSV-wave fields; (e) x- and (f) z-components of the total displacement fields.
Figure 10: Elastic wavefield extrapolation using 10th-order FD scheme and low-rank vector decomposition in SEG/Hess VTI model: (a) x- and (b) z-components of the synthetic elastic displacement wavefields at 1.1 s; (c) x- and (d) z-components of vector qP-wave fields; (e) x- and (f) z-components of vector qSV-wave fields.

Figure 11: Partial of BP 2007 TTI model with parameters of (a) vertical P-wave velocity, Thomsen coefficients (b) $\epsilon$ and (c) $\delta$, and (d) tilt angle $\theta$. 
Figure 12: Synthesized decoupled and total displacement fields at the time of 1.2 s using the low-rank pseudo-spectral solution with the $k$-space adjustment that simultaneously extrapolate and decouple qP- and qSV-wave fields in the BP 2007 TI model: (a) x- and (b) z-components of qP-wave fields; (c) x- and (d) z-components of qSV-wave fields; (e) x- and (f) z-components of the total displacement fields.
CONCLUSIONS

We have proposed a recursive integral method to simultaneously extrapolate and decompose the elastic wavefields on the basis of second-order displacement equation for heterogeneous anisotropic media. The computational efficiency is guaranteed by merging the operations of time extrapolation and vector decomposition into a unified Fourier integral framework and speeding up the solutions using the low-rank approximation. The use of the $k$-space adjustment permits larger time-steps without reducing accuracy or introducing instability in the low-rank pseudo-spectral scheme. The synthetic example shows that our method could produce dispersion-free decoupled and total elastic wavefields efficiently. We expect that the proposed approaches to extrapolate the decoupled elastic waves have great potential for applications such as elastic RTM and FWI of multicomponent seismic data acquired on land and at the ocean bottom. The focus for future work will be on the staggered-grid pseudo-spectral solution of the displacement-stress or velocity-stress equation for anisotropic media with strong heterogeneity and lower order of symmetry.

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APPENDIX A

COMPONENTS OF THE CHRIStOFFEL MATRIX

For a general anisotropic medium, the components of the density normalized Christoffel matrix $\Gamma$ are given as follows,

\[
\begin{align*}
\Gamma_{11} &= \left[ C_{11}k_x^2 + C_{66}k_y^2 + C_{55}k_z^2 + 2C_{56}k_yk_z + 2C_{15}k_xk_z + 2C_{16}k_xk_y \right]/\rho, \\
\Gamma_{22} &= \left[ C_{66}k_y^2 + C_{22}k_y^2 + C_{44}k_z^2 + 2C_{24}k_yk_z + 2C_{46}k_xk_z + 2C_{26}k_xk_y \right]/\rho, \\
\Gamma_{33} &= \left[ C_{55}k_z^2 + C_{44}k_y^2 + C_{33}k_z^2 + 2C_{34}k_yk_z + 2C_{35}k_xk_z + 2C_{45}k_xk_y \right]/\rho, \\
\Gamma_{12} &= \left[ C_{16}k_x^2 + C_{26}k_y^2 + C_{45}k_z^2 + (C_{46} + C_{25})k_yk_z + (C_{14} + C_{56})k_xk_z + (C_{12} + C_{65})k_xk_y \right]/\rho, \\
\Gamma_{13} &= \left[ C_{15}k_x^2 + C_{46}k_y^2 + C_{35}k_z^2 + (C_{45} + C_{36})k_yk_z + (C_{13} + C_{55})k_xk_z + (C_{14} + C_{56})k_xk_y \right]/\rho, \\
\Gamma_{23} &= \left[ C_{56}k_x^2 + C_{24}k_y^2 + C_{34}k_z^2 + (C_{44} + C_{23})k_yk_z + (C_{36} + C_{45})k_xk_z + (C_{25} + C_{46})k_xk_y \right]/\rho.
\end{align*}
\]
APPENDIX B

EXTENDED FORMULATIONS OF THE PSEUDO-SPECTRAL OPERATORS

According to equations 6 and 8, we express the pseudo-spectral operator that can be used to extrapolate the coupled elastic wavefields in its extended formation:

\[
\begin{align*}
    u_x(x, t + \Delta t) &= -u_x(x, t - \Delta t) + \int e^{ikx}w_{xx}(x, k)\tilde{u}_x(k, t) \, dk \\
    u_y(x, t + \Delta t) &= -u_y(x, t - \Delta t) + \int e^{ikx}w_{xy}(x, k)\tilde{u}_y(k, t) \, dk \\
    u_z(x, t + \Delta t) &= -u_z(x, t - \Delta t) + \int e^{ikx}w_{xz}(x, k)\tilde{u}_z(k, t) \, dk
\end{align*}
\]

(B-1)

in which \(\tilde{u}_x(k, t)\), \(\tilde{u}_y(k, t)\) and \(\tilde{u}_z(k, t)\) represent the three components of the elastic wavefields in wavenumber-domain at the time of \(t\).

For a VTI or orthorhombic medium, we express the stiffness tensor as a Voigt matrix:

\[
    C = \begin{pmatrix}
    C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
    C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
    C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\
    0 & 0 & 0 & C_{44} & 0 & 0 \\
    0 & 0 & 0 & 0 & C_{55} & 0 \\
    0 & 0 & 0 & 0 & 0 & C_{66}
    \end{pmatrix},
\]

(B-2)

in which there are only five independent coefficient with \(C_{12} = C_{11} - 2C_{66}, C_{22} = C_{11}, C_{23} = C_{13}\) and \(C_{55} = C_{44}\), for a VTI medium. Therefore, the propagation matrix has the following extended formulation,

\[
\begin{align*}
    w_{xx}(k) &= 2 - \Delta t^2[C_{11}k_x^2 + C_{66}k_y^2 + C_{55}k_z^2], \\
    w_{yy}(k) &= 2 - \Delta t^2[C_{66}k_x^2 + C_{22}k_y^2 + C_{44}k_z^2], \\
    w_{zz}(k) &= 2 - \Delta t^2[C_{55}k_x^2 + C_{44}k_y^2 + C_{33}k_z^2], \\
    w_{xy}(k) &= -\Delta t^2[C_{12} + C_{66}]k_xk_y, \\
    w_{xz}(k) &= -\Delta t^2[C_{13} + C_{55}]k_xk_z, \\
    w_{yz}(k) &= -\Delta t^2[C_{23} + C_{44}]k_yk_z.
\end{align*}
\]

(B-3)

If the principal axes of the medium are not aligned with the Cartesian axes, e.g., for the tilted TI and orthorhombic media, we should apply the Bond transformation [Winterstein, 1990; Carcione, 2007] to get the stiffness matrix under the Cartesian system. This will introduce more mixed partial derivative terms in the wave equation, which demands lots of computational effort if a finite-difference algorithm is used to extrapolate the wavefields. Fortunately, for the pseudo-spectral solution, it only introduces negligible computation to prepare the propagation matrix and no extra computation for the wavefield extrapolation.
Similarly, we can write the propagation matrix $\overline{w}_{ij}^{(m)}$ (in equation $20$) for the decoupled elastic waves in its extended formulation:

\[
\begin{align*}
\overline{w}_{xx}^{(m)}(x, k) & = d_{xx}^{(m)}(x, k)w_{xx}(x, k) + d_{xy}^{(m)}(x, k)w_{xy}(x, k) + d_{xz}^{(m)}(x, k)w_{xz}(x, k), \\
\overline{w}_{xy}^{(m)}(x, k) & = d_{xx}^{(m)}(x, k)w_{xy}(x, k) + d_{xy}^{(m)}(x, k)w_{yy}(x, k) + d_{xz}^{(m)}(x, k)w_{yz}(x, k), \\
\overline{w}_{xz}^{(m)}(x, k) & = d_{xx}^{(m)}(x, k)w_{xz}(x, k) + d_{xy}^{(m)}(x, k)w_{yy}(x, k) + d_{xz}^{(m)}(x, k)w_{yz}(x, k), \\
\overline{w}_{yx}^{(m)}(x, k) & = d_{yy}^{(m)}(x, k)w_{xy}(x, k) + d_{xy}^{(m)}(x, k)w_{yy}(x, k) + d_{yz}^{(m)}(x, k)w_{yz}(x, k), \\
\overline{w}_{yz}^{(m)}(x, k) & = d_{yy}^{(m)}(x, k)w_{yz}(x, k) + d_{xy}^{(m)}(x, k)w_{yy}(x, k) + d_{yz}^{(m)}(x, k)w_{yy}(x, k), \\
\overline{w}_{zz}^{(m)}(x, k) & = d_{zz}^{(m)}(x, k)w_{zz}(x, k) + d_{yz}^{(m)}(x, k)w_{yz}(x, k) + d_{xz}^{(m)}(x, k)w_{xz}(x, k), \\
\end{align*}
\]

\[(B-4)\]

**APPENDIX C**

**K-SPACE ADJUSTMENT TO THE PSEUDO-SPECTRAL SOLUTION**

According to the eigen-decomposition of the Christoffel matrix (see Equations 9 to 12), we can obtain the scalar wavefields for homogeneous anisotropic media using the theory of mode separation \([\text{Dellinger and Etgen} 1990]\),

\[
\hat{u}_i = Q_{ij} \hat{u}_j,
\]

\[(C-1)\]

in which $\hat{u}_i$ with $i = 1, 2, 3$ represents the scalar $qP$-, $qS_1$- and $qS_2$-wave fields. So these wavefields satisfy the same scalar wave equation

\[
\partial_t^2 \hat{u}_i + (v_i k)^2 \hat{u}_i = 0.
\]

\[(C-2)\]

The standard leapfrog scheme for this equation can be expressed as

\[
\frac{\hat{u}_i^{(n+1)} - 2\hat{u}_i^{(n)} + \hat{u}_i^{(n-1)}}{\Delta t^2} = -\lambda_i^{(n)} \hat{u}_i.
\]

\[(C-3)\]

It is well known that this solution is limited to small time-steps for stable wave propagation.

Fortunately, there is an exact time-stepping solution for the second-order time derivatives allowing for any size of time-steps for homogeneous medium \([\text{Cox et al. 2007}; \text{Etgen and Brandsberg-Dahl} 2009]\), namely:

\[
\frac{\hat{u}_i^{(n+1)} - 2\hat{u}_i^{(n)} + \hat{u}_i^{(n-1)}}{\Delta t^2} = -\sin^2(\lambda_i \Delta t/2) \frac{\hat{u}_i^{(n)}}{(\Delta t/2)^2}.
\]

\[(C-4)\]
Comparing equations C-3 and C-4 shows that, it is possible to extend the length of time-step without reducing the accuracy by replacing $(\lambda_i \Delta t/2)^2$ with $\sin^2 (\lambda_i \Delta t/2)$. This opens up a possibility by replacing $k^2$ with $k^2 \text{sinc}^2(\lambda_i \Delta t/2)$ as a $k$-space adjustment to the spatial derivatives, which may convert the time-stepping pseudo-spectral solution into an exact one for homogeneous media, and stable for larger time-steps (for a given level of accuracy) in heterogeneous media (Bojarski, 1982).

Nowadays, the $k$-space scheme is widely used to improve the approximation of the temporal derivative in acoustic and ultrasound (Tabei et al., 2002; Cox et al., 2007; Fang et al., 2014). As far as we know, Liu (1995) was the first to apply $k$-space ideas to elastic wave problems. He derived a $k$-space form of the dyadic Green’s function for the second-order wave equation and used it to calculate the scattered field iteratively in a Born series. Firouzi et al. (2012) proposed a $k$-space scheme on the base of the first-order elastic wave equation for isotropic media.

Accordingly, we apply the $k$-space adjustment to improve the performance of our two-step time-marching pseudo-spectral solution of the anisotropic elastic wave equation. To propagate the elastic waves on the base of equations 6 and 8, we need modify the eigenvalues of Christoffel matrix as in Equation 14.
REFERENCES

Fomel, S., L. Ying, and X. Song, 2013, Seismic wave extrapolation using lowrank symbol approximation: Geophysical Prospecting, 1–11.
Fowler, P., and R. King, 2011, Modeling and reverse time migration of orthorhom-


Propagate decoupled anisotropic elastic waves

Yan, J., and P. Sava, 2008, Isotropic angle domain elastic reverse time migration: Geophysics, 73, S229–S239.
Fast algorithms for elastic-wave-mode separation and vector decomposition using low-rank approximation for anisotropic media

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ABSTRACT

Wave mode separation and vector decomposition are significantly more expensive than wavefield extrapolation and are the computational bottleneck for elastic reverse-time migration (ERTM) in heterogeneous anisotropic media. We express elastic wave mode separation and vector decomposition for anisotropic media as space-wavenumber-domain operations in the form of Fourier integral operators, and develop fast algorithms for their implementation using their low-rank approximations. Synthetic data generated from 2D and 3D models demonstrate that these methods are accurate and efficient.

INTRODUCTION

Seismic waves are described by the elastic wave equation with P- and S-waves intrinsically coupled. An elastic migration or inversion program should be able to handle both wave modes. Normally the P and S modes are separated and each is treated independently. Otherwise, the two modes are mixed on all wavefield components and cause crosstalk and image artifacts (Yan and Sava, 2009b). In isotropic media, farfield P- and S-wave modes can be separated by taking the divergence and curl in the extrapolated elastic wavefield. It is well known that a shear wave passing through an anisotropic medium can split into two mutually orthogonal waves (Crampin 1984). Generally the P-wave and the two S-waves in anisotropic materials are not polarized parallel and perpendicular to the wave vectors and can not be fully separated with divergence and curl operations.

To account for seismic anisotropy, wave mode separation concept and approach have been extended in the past two decades. Dellinger and Etgen (1990) generalize divergence and curl to anisotropic media by constructing the separators in the wavenumber domain, and independently solving the Christoffel equation in each wave propagation direction. For heterogeneous media, these divergence-like and curl-like separators are rewritten by Yan and Sava (2009b) as nonstationary spatial filters determined by the local polarization vectors. Zhang and McMechan (2010) develop a wavefield decomposition method to separate elastic wavefields into vector P- and
S-wave fields for vertically transverse isotropic (VTI) media. Alternatively, we may implicitly achieve partial mode separation during wavefield extrapolation using the so-called pseudo-pure-mode wave equations, and then obtain completely separated wave modes by correcting the polarization projection deviation of the pseudo-pure-mode wavefields from the isotropic reference \cite{Cheng2012, Cheng2013}. Although these studies provide significant insights into wave mode separation in anisotropic media, many challenges remain, especially in the computational implementation if the proposed approaches are directly used in practice. For example, mode separation using nonstationary filtering is computationally expensive, especially in 3D. To improve efficiency, Yan and Sava \cite{Yan2011} present a mixed-domain algorithm that resembles the phase-shift plus interpolation (PSPI) scheme from one-way wave equation migration \cite{Gazdag1984}. The compromise between accuracy and cost requires to determine the minimal reference models that best represent the true model space, and the choice of the models is case dependent. On the other hand, Zhang and McMechan \cite{Zhang2010}'s wavenumber-domain vector decomposition approach is effective when the model can be separated into distinct geologic units. In addition, spectral methods were proposed to provide solutions which can completely avoid the crosstalk between the qP and qS modes in wavefield modeling and reverse-time migration (RTM) \cite{Etgen2009, Liu2009, Chu2011, Pestana2011, Fomel2013, Song2013}. However, these pure-mode solutions fail to provide accurate amplitudes for qP- and qS-waves. For true-amplitude ERTM in anisotropic media, effective mode separation and decomposition are highly required before applying the imaging condition to the extrapolated elastic wavefields \cite{Zhang2011}.

In this paper, we respectively propose fast algorithms for elastic wave mode separation and vector decomposition in 3D heterogeneous transverse isotropic (TI) media. First, we give a brief review of the underlying principles. Then we present space-wavenumber-domain operations for mode separation and vector decomposition in the form of Fourier integral operators, and discuss how to construct efficient algorithms using low-rank approximation \cite{Engquist2008}. At the end, we test efficiency and accuracy of the proposed method using synthetic models of increasing complexity.

**ELASTIC WAVE MODE SEPARATION**

Using the Helmholtz decomposition theory \cite{Morse1953, Aki1980}, a vector wavefield $\mathbf{U} = \{U_x, U_y, U_z\}$ can be decomposed into a curl-free P-wavefield and a divergence-free S-wavefield: $\mathbf{U} = \mathbf{U}^P + \mathbf{U}^S$. The P- and S-waves satisfy, respectively,

$$\nabla \times \mathbf{U}^P = 0, \quad \text{and} \quad \nabla \cdot \mathbf{U} = \nabla \cdot \mathbf{U}^P,$$ \hspace{1cm} (1)

and

$$\nabla \cdot \mathbf{U}^S = 0, \quad \text{and} \quad \nabla \times \mathbf{U} = \nabla \times \mathbf{U}^S.$$ \hspace{1cm} (2)
These equations imply that the divergence and curl operations pass P- and S-wave modes respectively. In the Fourier-domain, equivalent operations are expressed as follows:

$$\tilde{P}(k) = ik \cdot \tilde{U}(k), \quad \text{and} \quad \tilde{S}(k) = ik \times \tilde{U}(k),$$

(3)

where $$k = \{k_x, k_y, k_z\}$$ represents the wave vector and $$\tilde{U}(k)$$ is the 3D wavefield in the wavenumber domain. These operations essentially project the elastic wavefield onto the wave vector or its orthogonal directions, thus separate P- and S-waves successfully. In anisotropic media, however, qP- and qS-waves are not generally polarized parallel and perpendicular to the wave vector. Dellinger and Etgen (1990) extended wave mode separation to anisotropic media with the following divergence-like and curl-like operators in the wavenumber-domain,

$$\tilde{qP}(k) = i\tilde{a}_p(k) \cdot \tilde{U}(k), \quad \text{and} \quad \tilde{qS}(k) = i\tilde{a}_p(k) \times \tilde{U}(k),$$

(4)

where $$\tilde{a}_p(k)$$ stands for the normalized polarization vector of qP wave in the wavenumber domain, calculated from Christoffel equation. Note that the second equation of equation 4 separates only the shear part of the elastic wavefields, which contain the fast and slow S-waves, i.e., qS1- and qS2 modes. Unlike the well-behaved qP mode, the two qS modes do not consistantly polarize as a function of the propagation direction (or wavenumber) and thus cannot be designated as SV and SH waves, except in isotropic and TI media (Winterstein 1990; Crampin 1991; Dellinger 1991; Zhang and McMechan 2010). In this paper, the approaches to separate and decompose qS-waves are restricted to TI anisotropy.

For TI media, one can separate scalar qSV and SH waves by projecting the elastic wavefield onto their polarization directions using

$$\tilde{qSV}(k) = i\tilde{a}_{sv}(k) \cdot \tilde{U}(k), \quad \text{and} \quad \tilde{SH}(k) = i\tilde{a}_{sh}(k) \cdot \tilde{U}(k),$$

(5)

where $$\tilde{a}_{sv}(k)$$ and $$\tilde{a}_{sh}(k)$$ represent normalized polarization vectors of the qSV and SH waves, respectively. For heterogeneous TI media, these operations can be expressed as nonstationary filtering in the space domain (Yan and Sava 2009b). In fact, the cost may become prohibitive in 3D because it is proportional to the number of grids in the model and the size of each filter (Yan and Sava 2011).

In general, we can determine polarization vectors by solving the Christoffel equation:

$$\tilde{G} - \rho V_n^2 \mathbf{I} \tilde{a}_n = 0,$$

(6)

where $$\tilde{G}$$ represents the Christoffel tensor in the Voigt notation with $$\tilde{G}_{ij} = c_{ijkl}n_j n_l$$ as the stiffness tensor, and $$n_j$$ and $$n_l$$ are the normalized wave vector components in j and l directions, with $$i, j, k, l = 1, 2, 3$$. The parameter $$V_n(n = qP, qS_1, qS_2)$$ represents phase velocities of qP-, qS1- and qS2-wave modes. The Christoffel equation poses a standard 3 x 3 eigenvalue problem, the three eigenvalues of which correspond to phase velocities of the three wave modes and the corresponding eigenvector $$\tilde{a}_n$$ represents polarization direction of the given mode. When shear singularities appear, the coincidence of the longitudinal and transverse polarizations prevents us from constructing
3D global operators to separate qSV and SH waves on the base of the Christoffel solution, and the polarization discontinuity will cause the two modes to leak energy into each other (Dellinger, 1991; Yan and Sava, 2009a; Zhang and McMechan, 2010; Yan and Sava, 2011). Following Yan and Sava (2009a, 2011), we mitigate the kiss singularity at $k_z = \pm 1$ in 3D TI media by using relative qP-qSV-SH mode polarization orthogonality and scaling the polarizations of the qSV- and SH-waves by $\sin \phi$, with $\phi$ being the polar angle.

**ELASTIC WAVE VECTOR DECOMPOSITION**

Wavefield decomposition aims achieving mode separation and vector decomposition simultaneously. On the base of the Helmholtz theory and the theory of anisotropic wave mode separation via the Christoffell equation, Zhang and McMechan (2010) develop a new solution to the problem of decomposing an elastic wavefield into P- and S-waves for isotropic and VTI media. We summarize here only their results used for this study.

For isotropic media, the Helmholtz equations for the P-wave are transformed into the wavenumber-domain as,

$$k \times \tilde{U}^P = 0, \quad \text{and} \quad k \cdot \tilde{U} = k \cdot \tilde{U}^P.$$

(7)

From these equations, the vector decomposition equation of the separated P-wave is given by:

$$\tilde{U}^P(k) = \tilde{k} [k \cdot \tilde{U}(k)].$$

(8)

where $\tilde{k}$ represents the normalized wave vector.

In a TI medium, equation 8 is extended to separate and decompose qP-wave by substituting $a_p$ for $k$,

$$\tilde{U}^{qP}(k) = a_p(k) [a_p(k) \cdot \tilde{U}(k)].$$

(9)

Similar equations

$$\tilde{U}^{qSV}(k) = a_{sv}(k) [a_{sv}(k) \cdot \tilde{U}(k)],$$

(10)

and

$$\tilde{U}^{SH}(k) = a_{sh}(k) [a_{sh}(k) \cdot \tilde{U}(k)],$$

(11)

are proposed to decompose qSV and SH waves using their respective polarization vectors. Note that vector decomposition satisfies the linear superposition relation $\tilde{U} = \tilde{U}^{qP} + \tilde{U}^{SH} + \tilde{U}^{qSV}$, and the separated wavefields are orthogonal to one another and have the same amplitude, phase, and physical units as the input wavefields.

**LOW-RANK APPROXIMATION SOLUTIONS**

We observe that both elastic wave mode separation and vector decomposition are based on polarization of wave modes, and any wave mode shares the algorithm structure of separation or decomposition. We will use qP-wave as an example.
We first write the equivalent version of the first equation of equation 4 in the space-domain as

$$ q_P(x) = \int e^{i k x} \left[ i a_{px}(k) \tilde{U}_x(k) + i a_{py}(k) \tilde{U}_y(k) + i a_{pz}(k) \tilde{U}_z(k) \right] dk. \quad (12) $$

To tackle spatial variations of the polarization in heterogeneous media, we extend the integral operators using

$$ q_P(x) = \int e^{i k x} \left[ i a_{px}(x, k) \tilde{U}_x(k) \right] dk + \int e^{i k x} \left[ i a_{py}(x, k) \tilde{U}_y(k) \right] dk + \int e^{i k x} \left[ i a_{pz}(x, k) \tilde{U}_z(k) \right] dk, \quad (13) $$

where $a_{px}(x, k)$, $a_{py}(x, k)$ and $a_{pz}(x, k)$ represent the $x$-, $y$- and $z$-components of the normalized polarization vector of $qP$ waves at location $x$. Compared with nonstationary filtering (Yan and Sava, 2009b), these pseudospectral-like operations are more accurate but less efficient. The computation complexity of the straightforward implementation is $O(N_x^2)$, which is prohibitively expensive when the size of model $N_x$ is large.

Similarly, from equation 9, we can derive the space-wavenumber-domain operators for decomposing $qP$-waves. For example, the $x$-component of $qP$-wave satisfies,

$$ U_{qP}^x(x) = \int e^{i k x} \left[ a_{px}(x, k) a_{px}(x, k) \right] \tilde{U}_x(k) dk + \int e^{i k x} \left[ a_{px}(x, k) a_{py}(x, k) \right] \tilde{U}_y(k) dk + \int e^{i k x} \left[ a_{px}(x, k) a_{pz}(x, k) \right] \tilde{U}_z(k) dk, \quad (14) $$

Note that more multiplication operations are needed for vector decomposition.

The discrete implementation of each integral operation in equation 13 or 14 naturally arises as a numerical approximation of a continuous Fourier integral operator (FIO) of the general form. Underlying fast solutions to FIOs is a mathematical insight concerning restriction of the integral kernel to subsets of space and wavenumber domains. Whenever these subsets obey a simple geometric condition, the restricted kernel is approximately low rank (Candes et al., 2007; Ying, 2012). Recently, several two-way wave extrapolation operators have been developed with the help of a low-rank approximation of the space-wavenumber-domain wave-propagator matrix in variable and possibly anisotropic media (Fomel et al., 2010, 2013; Song et al., 2011; Song and Alkhalifah, 2013; Alkhalifah, 2013).

For both mode separation and vector decomposition, phase terms in the FIOs are relatively simple and can be absorbed into inverse Fourier transforms. Therefore our main task is to respectively construct low-rank decomposition for the amplitude terms in the kernel. Previously, Fomel et al. (2013) applied low-rank approximation to the phase-only terms in wave extrapolation operators. Any amplitude term bracketed in equations 13 and 14 can be approximated by the following separated representation:

$$ W_j(x, k) \approx \sum_{m=1}^M \sum_{n=1}^N B(x, k_m) A_{mn} C(x_n, k), \quad (15) $$
in which \( j = x, y, z \), \( N \) and \( M \) represent the rank of this decomposition, \( W_j(x, k) \) represents the mixed-domain mode separation or vector decomposition operator, \( B(x, k_m) \) is a mixed-domain matrix with reduced wavenumber dimension, \( C(x_n, k) \) is a mixed-domain matrix with reduced spatial dimension, and \( A_{mn} \) is a \( M \times N \) matrix. The construction of the separated form \( 15 \) follows the method of Engquist and Ying (2009). It can be viewed as a matrix decomposition problem, i.e.,

\[
W \approx BC,
\]

where \( W \) is the \( NxN \) matrix with entries \( W_j(x, k) \), \( B \) is the submatrix of \( W \) that consists of columns associated with \( \{k_m\} \), \( C \) is the submatrix that consists of rows associated with \( \{x_n\} \), and \( A = \{A_{mn}\} \). Physically, a separable low-rank approximation amounts to selecting a set of \( N (N \ll N_x) \) representative spatial locations and \( M (M \ll N_x) \) representative wavenumbers. As explained by Fomel et al. (2013) in detail, we first need to restrict the mixed-domain \( W \) to \( n \) randomly selected rows. In practice, \( n \) can be scaled as \( O(r \log N_x) \) and \( r \) represents the numerical rank of \( W \). Then we apply pivoted QR algorithm (Golub and Loan, 1996) to find the corresponding columns for \( B(x, k_m) \). To find the rows for \( C(x_n, k) \), we apply the pivoted QR algorithm to \( W^* \). The algorithm does not require, at any step, access to the full-matrix \( W \), only to its selected rows and columns.

Representation \( 15 \) speeds up the computation of the FIOs in equations \( 13 \) and \( 14 \) since

\[
\int e^{ikx}W_j(x, k)\tilde{U}_j(k)\,dk \approx \\
\sum_{m=1}^{M} B(x, k_m) \left( \sum_{n=1}^{N} a_{mn} \left( \int e^{ikx}C(x_n, k)\tilde{U}_j(k)\,dk \right) \right),
\]

The evaluation of the last formula is effectively equivalent to applying \( N \) inverse fast Fourier transforms (FFTs). Accordingly, with low-rank approximation, the computation complexity reduces to \( O(NN_x \log N_x) \). In other word, the costs are mainly controled by the model size \( N_x \) and the rank \( N \), which depends on the complexity of the anisotropic velocity model. For isotropic models with arbitrary heterogeneity, the rank automatically reduces to 1 because the polarization directions are material-independent. Similarly to the observation by Fomel et al. (2013), there is a natural tradeoff in the selection of \( N \): larger values lead to a more accurate separated representation but require a longer computational time. In the examples of the next section, the ranks are automatically calculated based on the estimate of the approximation accuracy and generally aiming for the relative single-precision accuracy (namely the maximum allowable error in low-rank decomposition) of \( 10^{-6} \). In multiple-core implementations, the matrix operations in equation \( 17 \) are easy to parallelize.

For some applications such as ERTM in TI media, one should construct the separated representations of the operator matrixes in advance, and then implement mode separation or/decomposition of the extrapolated elastic wavefields before applying the imaging condition. To further save computational cost, appropriate relaxing of
the accuracy requirement for low-rank approximation and applying mode separation only every two or three time steps are both good choices in practice.

EXAMPLES

This section contains four examples. They are for 2D and 3D two-layer models, the SEG/Hess VTI model and the BP 2007 TTI model, respectively. We use 10th-order finite-difference algorithm for elastic wavefield extrapolation. To accurately compare the used CPU times, algorithm parallelization is not considered for wave mode separation and vector decomposition.

A 2D two-layer TI model

We first test our approach on a two-layer TI model with the size of $N = 401 \times 401$. The first layer is a VTI medium with $v_p = 2500 \text{ m/s}$, $v_s = 1200 \text{ m/s}$, $\epsilon = 0.25$, and $\delta = -0.25$, and the second layer is a TTI medium with $v_p = 3600 \text{ m/s}$, $v_s = 1800 \text{ m/s}$, $\epsilon = 0.2$, $\delta = 0.1$, and the tilt angle $\theta = 30^\circ$. A point-source is placed at the center of this model. To aim for the relative accuracy, rank $N = M = 2$ is required for both mode separation and vector decomposition. Thanks to small approximation errors in low-rank decompositions (see Figures 1 and Figure 3), we obtain good mode separation and vector decomposition for the synthesized elastic wavefields (see Figures 2 and 4). It took CPU time of 7.5 seconds to construct the separated forms (as equation 15 expressed) of the mode separation matrixes for qP- and qSV-waves. For one time step, it took CPU time of 0.12, 0.21, and 0.33 seconds to extrapolate, separate and decompose the elastic wavefields, respectively.

A 3D two-layer TI model

We also test the mode separation approach on a 3D two-layer TI model, with $v_p = 2500 \text{ m/s}$, $v_s = 1200 \text{ m/s}$, $\epsilon = 0.25$, $\delta = -0.25$ and $\gamma = 0$ in the first layer, and $v_p = 3600 \text{ m/s}$, $v_s = 1800 \text{ m/s}$, $\epsilon = 0.2$, $\delta = 0.1$ and $\gamma = 0.05$ in the second layer. The size of the model is $N = 201 \times 201 \times 201$. A displacement source located at the center of the model and oriented at tilt $45^\circ$ and azimuth $45^\circ$. Figure 5 displays the elastic wavefields and the separated qP-, qSV- and SH-wave fields using the low-rank approximate algorithm. Because the substantial increase of the model size, it is still time consuming to separate the 3D wave modes even if the proposed fast algorithm is used. It took 4008.0, 4130.0 and 91.8 seconds to construct the separated forms of the mode separation matrixes for qP-, qSV- and SH-waves, respectively. For one time step, it took 61.4 seconds to extrapolate the elastic wavefield, and 15.2, 15.8 and 6.8 seconds to separate qP-, qSV- and SH-wave fields with the rank $N = M = 2$.

For comparison, we only change the second layer to a TTI medium with a tilt angle $\theta = 30^\circ$ and azimuth $\phi = 30^\circ$ (other parameters continue to use). Figure 6 displays the
corresponding elastic wavefields and their mode separation results. It took 4087.8, 4280.8 and 206.2 seconds to construct the separated forms of the mode separation matrices for qP-, qSV- and SH-waves, respectively. For one time step, it took 101.0 seconds to extrapolate the elastic wavefield, and 15.2 and 15.8 seconds to separate qP- and qSV-wave modes with the rank $N = M = 2$. It took 14.1 seconds to separate SH-wave with the rank $N = M = 2$. As we observed, the most time-consuming task here is to construct the separated forms of the mode separation matrices. More CPU time is required to separate SH-wave in 3D TTI media as well.

**SEG Hess VTI model**

Then we demonstrate the approach in the 2D Hess VTI model (Figure 7). Vertical S-wave velocity is set to equal half the vertical P-wave velocity everywhere. A point-source is placed at location of (13.264, 4.023) km. Figure 7 shows results of mode separation and vector decomposition, with the rank of about 6 in both cases. It took 133.0 seconds to decompose the operator matrixes for mode separation with rank $N = M = 6$, and 154.1 seconds to decompose the operator matrixes for vector decomposition with rank $N, M \in [6, 7]$. For one time step, it took about 2.2, 4.0, and 7.7 seconds to extrapolate, separate and decompose the elastic wavefields, respectively. However, if nonstationary spatial filtering is used to separate qP- and qSV-waves at every grid-point, it took about 2340.7 seconds to calculate the filters in advance, and about 444.0 seconds with the truncated operator of size $51 \times 51$ at each time step during wavefield extrapolation. This indicates that the mixed domain algorithms using low-rank approximation significantly improve the efficiency for wave mode separation. Of course, larger amount of CPU time has been saved for vector decomposition by using the corresponding low-rank approximate algorithm.

**BP 2007 TTI model**

This example displays the wave mode separation and vector decomposition results in the BP 2007 TTI model (Figure 9). A point-source is placed near the second salt body at the location of (35.625, 5.0) km. Before wavefield extrapolation, separated representations of the operator matrixes are constructed using the low-rank decomposition approach within the computational zone. It took 217.0 seconds to decompose the operator matrixes for mode separation with rank $N, M \in [15, 17]$, and 345.5 seconds to decompose the operator matrixes for vector decomposition with rank $N, M \in [16, 18]$. For one time step, it took 4.3, 16.0 and 34.8 seconds to extrapolate, separate and decompose the elastic wavefields, respectively. From the separated and decomposed wavefields (Figure 10), we can clearly observe the converted waves from the dipping salt flanks. Due to the low velocities of qSV-wave in some directions at some locations, there are numerical dispersion in the qSV-wave fields. In spite of the dispersion, we obtain well separated qP- and qSV-wave fields, as well as their decomposed x- and z-components.
Figure 1: Low-rank approximate mode separators of qP-wave in a 2D two-layer TI model: (a) $a_{px}(x,k)$ and (b) $a_{pz}(x,k)$ constructed by using low-rank decomposition in the VTI layer; (c) $a_{px}(x,k)$ and (d) $a_{pz}(x,k)$ constructed by using low-rank decomposition in the TTI layer; (e), (f), (g) and (h) represent the low-rank approximation errors of these operators. According to the qP-qSV mode polarization orthogonality, we have the following relations: $a_{svx}(x,k) = -a_{pz}(x,k)$ and $a_{svz}(x,k) = a_{px}(x,k)$. Therefore, the above pictures also demonstrate the low-rank approximate separators and their errors for qSV-wave.
Figure 2: Elastic wave mode separation in the two-layer TI model: (a) x- and (b) z-components of the synthetic elastic displacement wavefields synthesized at 0.3s; (c) and (d) are the separated scalar qP- and qSV-wave fields using low-rank approximation.
Figure 3: Low-rank approximate vector decomposition operators of qP-wave in the 2D two-layer TI model: (a) $a_{px}(x,k)a_{px}(x,k)$, (b) $a_{pz}(x,k)a_{pz}(x,k)$, and (c) $a_{px}(x,k)a_{pz}(x,k)$, and (e), (f) and (g) represent their low-rank approximation errors in the VTI layer. (h), (i), (j), (k), (l) and (m) are these operators and their low-rank approximation errors in the TTI layer.
Figure 4: Elastic wave vector decomposition in the two-layer VTI/VTI model: (a) x- and (b) z-components of vector qP-wave fields; (c) x- and (d) z-components of vector qSV-wave fields.
Figure 5: Elastic wave mode separation in the 3D two-layer VTI model: (a) x-, (b) y- and (c) z-components of the synthetic elastic displacement wavefields synthesized at 0.17s; (d) qP-, (e) qSV- and (e) SH-wave fields separated from the elastic wavefields.
Figure 6: Elastic wave mode separation in the 3D two-layer VTI/TTI model: (a) x-, (b) y- and (c) z-components of the synthetic elastic displacement wavefields synthesized at 0.17s; (d) qP-, (e) qSV- and (e) SH-wave fields separated from the elastic wavefields.
Then we investigate the effect of the relative accuracy requirement on wave mode separation. Figure 11 demonstrates the separated P- and qSV-wave fields, and their variations when we relax the approximation level from $10^{-6}$ to $10^{-3}$. It took 174.0 seconds to decompose the operator matrixes for mode separation with rank $N, M \in [7, 8]$, and 345.5 seconds to decompose the operator matrixes for vector decomposition with rank $N, M \in [8, 9]$. And it took 8.0 and 14.9 seconds to separate and decompose the elastic wavefields, respectively. The results are acceptable although more errors are introduced in the separated wavefields when we turn down the relative accuracy requirement.

To further analyze the rough relationship of rank $(N, M)$ with the model complexity, we smooth the BP TTI model by applying a 2D triangle smoothing operator with the radius of 1875m on both x- and z-axes (Figure 12). To maintain the range of the tilt angles, we first double the values of the original model and then apply the smoothing operation for this parameter. Figure 13 demonstrates the synthetic elastic wavefields and the mode separation and vector decomposition results. In this case, it took 207.0 seconds to decompose the operator matrixes for mode separation with rank $N, M \in [13, 14]$, and 310.2 seconds to decompose the operator matrixes for vector decomposition with rank $N, M \in [14, 16]$. It took 15.0 and 29.4 seconds to separate and decompose the elastic wavefields, respectively. We observe that the ranks further decrease to about 12 if we double the smoothing radius to 3750m. For homogeneous TI medium, the ranks automatically decrease to 1. We obtain accurate mode separation and decomposition of the isotropic and elastic wavefields at negligible computational cost with rank $N = M = 1$, if $\epsilon$, $\delta$ and $\theta$ are all set as 0.0 in the models.
Figure 8: Elastic wave mode separation and vector decomposition in the Hess VTI model: (a) x- and (b) z-components of the synthetic elastic displacement wavefields at 1.1s; (c) and (d) are the separated scalar qP- and qSV-wave fields; (e) x- and (f) z-components of vector qP-wave fields; (g) x- and (h) z-components of vector qSV-wave fields.
Figure 9: BP 2007 TTI model with parameters of (a) vertical P-wave velocity, Thomsen coefficients (b) $\epsilon$ and (c) $\delta$, and (d) tilt angle $\theta$.

CONCLUSIONS AND DISCUSSION

We have developed two fast algorithms for wave mode separation and vector decomposition for heterogeneous TI media. They are based on the low-rank approximation of the space-wavenumber-domain operators, and reduces the cost to that of a small number of FFT operations per time step, corresponding to the approximation rank times the number of components. Synthetic examples show that our approach have high accuracy and efficiency. In general TI media, the rank increases when the models become complex but is always far smaller than the model size. For the 3D elastic wave mode separation and decomposition in heterogeneous TI media, however, constructing the separated representations of the mixed-domain operator matrixes is still time consuming due to the substantial increase of the model size. Parallelizing the algorithm for this procedure may provide a practical solution.

The key concepts of mode separation and vector decomposition are based on polarizations. Unlike the well-behaved P-wave mode, the S-wave modes do not consistently polarize as a function of the propagation direction, and thus can not be designated as SV and SH waves, except in isotropic and TI media. For a 3D TI medium, the effects of kiss singularity are mitigated by using the mutual orthogonality among the $qP$, $qSV$ and SH modes. This procedure only ensures that the two S-modes are accurately separated in kinematics. It is a challenge to find the right solution of the singularity problem and obtain completely separated two S-modes with correct
Figure 10: Mode separation and vector decomposition using low-rank approximate algorithms in the BP 2007 TTI model: (a) x- and (b) z-components of the synthetic elastic displacement wavefields at 1.4s; (c) and (d) are the separated scalar qP- and qSV-wave fields; (e) x- and (f) z-components of vector qP-wave fields; (g) x- and (h) z-components of vector qSV-wave fields.
Figure 11: Elastic wave mode separation using low-rank approximation with relaxed accuracy requirements: Separated (a) qP- and (b) qSV-wave fields at the error level of $10^{-3}$ in low-rank decomposition; Differences of (c) qP- and (d) qSV-wave fields to those separated with the error level of $10^{-6}$. 

[link](lrmode/bptti2007.comparison/ ElasticSepP3,ElasticSepSV3,ElasticSepP6vs3Dif,ElasticSepSV6vs3Dif)
Figure 12: Smoothed BP 2007 TTI model with parameters of (a) vertical P-wave velocity, Thomsen coefficients (b) \( \epsilon \) and (c) \( \delta \), and (d) tilt angle \( \theta \). 2D triangle smoothing with the smoothing radius of 1875m on both axis is applied to the parameters shown in Figure 9.

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REFERENCES


Figure 13: Mode separation and vector decomposition using low-rank approximate algorithms in the BP 2007 TTI model: (a) x- and (b) z-components of the synthetic elastic displacement wavefields at 1.4s; (c) and (d) are the separated scalar qP- and qSV-wave fields; (e) x- and (f) z-components of vector qP-wave fields; (g) x- and (h) z-components of vector qSV-wave fields.
———, 2013, Simulating propagation of separated wave modes in general anisotropic media, part I: P-wave propagators: Geophysics, 79.
———, 2013, Seismic wave extrapolation using lowrank symbol approximation: Geophysical Prospecting, 61, 526–536.
Winterstein, D., 1990, Velocity anisotropy terminology for geophysicists: Geophysics,
Anisotropic wave mode separation

Yan, J., and P. Sava, 2009a, 3D elastic wave mode separation for TTI media: SEG Technical Program Expanded Abstracts, 4294–4298.


Simulating propagation of separated wave modes in general anisotropic media, Part II: qS-wave propagators

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ABSTRACT

Shear waves, especially converted modes in multicomponent seismic data, provide significant information that allows better delineation of geological structures and characterization of petroleum reservoirs. Seismic imaging and inversion based upon the elastic wave equation involve high computational cost and many challenges in decoupling the wave modes and estimating so many model parameters. For transversely isotropic media, shear waves can be designated as pure SH and quasi-SV modes. Through two different similarity transformations to the Christoffel equation aiming to project the vector displacement wavefields onto the isotropic references of the polarization directions, we derive simplified second-order systems (i.e., pseudo-pure-mode wave equations) for SH- and qSV-waves, respectively. The first system propagates a vector wavefield with two horizontal components, of which the summation produces pure-mode scalar SH-wave data, while the second propagates a vector wavefield with a summed horizontal component and a vertical component, of which the final summation produces a scalar field dominated by qSV-waves in energy. The simulated SH- or qSV-wave has the same kinematics as its counterpart in the elastic wavefield. As explained in our previous paper (part I), we can obtain completely separated scalar qSV-wave fields after spatial filtering the pseudo-pure-mode qSV-wave fields. Synthetic examples demonstrate that these wave propagators provide efficient and flexible tools for qS-wave extrapolation in general transversely isotropic media.

INTRODUCTION

Ultrasonic laboratory studies as well as seismic field investigations have shown that many geological materials and subsurface structures are elastically anisotropic. It is well known that a shear wave passing through an anisotropic material splits into two mutually orthogonal waves, which propagate at different velocities. Therefore, seismic waves propagate through the earth as a superposition of three body wave modes, one P-wave and two S-waves. Generally they are polarized neither parallel to nor perpendicular to the direction of wave travel, thus are called quasi-P (qP) and quasi-S (qS) waves, with quasi- means similar to but not exactly. P- and S-waves were originally named for their arrival times, with P for the first (primary) and S
for the second. Today, the indicators P and S are often connected with polarization, i.e., P with compressional (or longitudinal) and S with shear (or transverse), with the specification SH and SV for waves with transverse displacements in the horizontal and vertical planes, respectively (Winterstein, 1990). For vertical transversely isotropic (VTI) media, one often uses this terminology with qP, qSV, and SH, since the first two of these waves are generally not purely longitudinal and transverse, respectively.

Because seismic anisotropy by nature is an elastic phenomenon, the full elastic wave equation is usually more accurate for wavefield extrapolation than the acoustic equation. However, seismic imaging using the elastic wave equation involve high computational cost and many challenges in decoupling wave modes to get physically interpretable images of the subsurface (Dellinger and Etgen, 1990; Zhang and McMechan, 2010; Yan and Sava, 2011; Cheng and Fomel, 2014). For real-sized applications of seismic imaging and inversion, it is necessary to resort to a simplified description of wave propagation in anisotropic media.

Pseudoacoustic wave equations are the most common approximations made to mono-component (mainly pressure) seismic data. They are derived by setting the qS-wave phase velocity along the symmetry axis to zero for VTI or orthorhombic media (Alkhalifah, 2000, 2003; Duveneck and Bakker, 2011). Pseudoacoustic wave equations describe the kinematic signatures of qP-waves with sufficient accuracy and are simpler than their elastic counterparts, which leads to computational savings in practice (Zhou et al., 2006; Fletcher et al., 2009; Zhang and Zhang, 2011). They also have fewer parameters, which is important for inversion. However, we note several limitations of the acoustic anisotropic wave equation. First, acoustic approximation does not prevent the propagation of qS-waves in directions other than the symmetry axis (Grechka et al., 2004; Zhang et al., 2005); the residual qS-waves are regarded as artifacts in the framework of acoustic modeling, reverse-time migration (RTM) and full waveform inversion (FWI) (Alkhalifah, 2000; Zhang et al., 2009; Operto et al., 2009). Second, stability analysis based on requiring the stiffness tensor to remain positive definite (Helbig, 1994) shows that wavefield extrapolation in a pseudo-acoustic TI or orthorhombic medium can become unstable (Alkhalifah, 2000; Grechka et al., 2004; Fowler and King, 2011). Alternatively, qP- and qS-wave propagation can be formally decoupled in the wavenumber domain to yield pure-mode pseudodifferential equations (Liu et al., 2009; Du et al., 2014). Unfortunately, these equations in time-space domain cannot be solved with traditional numerical schemes. Through factorizing and approximating the qP-qSV dispersion relations or phase velocities, many authors proposed to simulate propagation of scalar pure-mode waves using mixed-domain recursive integral operators (Etgen and Brandsberg-Dahl, 2009; Liu et al., 2009; Zhang and Zhang, 2009; Crawley et al., 2010; Fowler et al., 2010; Chu et al., 2011; Pestana et al., 2011; Zhan et al., 2012; Fomel et al., 2013) or novel finite-difference operators (Song et al., 2013). To avoid solving the pseudodifferential equation, Xu and Zhou (2014) proposed a nonlinear wave equation for a pseudo-acoustic qP-wave with an auxiliary scalar operator depending on the material parameters and the phase direction of the propagation at each spatial location.
Multicomponent seismic data are increasingly acquired on land and at the ocean bottom to better delineate geological structures and to characterize oil and gas reservoirs (Li, 1997; Thomsen, 1999; Cary, 2001; Stewart et al., 2002; Hardage et al., 2011). The development of unconventional reservoirs and the microseismic monitoring of hydraulic fracturing has led to more interest in shear waves because microseismic sources emit strong shear energy that is routinely recorded by three-component geophones (Maxwell, 2010) and is widely recognized as being useful for locating microseismic events and estimating their focal mechanisms (Baig and Urbancic, 2010; Grechka and Yaskevich, 2014). In fact, anisotropic phenomena are especially noticeable in shear and mode-converted wavefields. Therefore, modeling of anisotropic shear waves may be important both theoretically and practically. As we know, the pseudoacoustic approximation is not appropriate for qS-waves. In addition to amplitude errors, the kinematic accuracy of qS-waves is reduced if we use the existing numerical schemes based on factorizing and approximating the dispersion relations or phase velocities.

In kinematics, there are various forms equivalent to the original elastic wave equations. In our previous paper (part I), we derived the pseudo-pure-mode wave equation for qP-waves by applying a particular similarity transformation to the Christoffel equation and demonstrated its features in describing wave propagation for TI and orthorhombic media. Except for its application to scalar qP-wave RTM (Cheng and Kang, 2014), the pseudo-pure-mode wave equation provides new insight into developing approaches for multicomponent qP-wave inversion (Djebbi and Alkhalifah, 2014). The same theoretical framework described in part I is applied to qS-waves in this paper. First we derive the pseudo-pure-mode wave equations for qS-waves in TI media through new similarity transformations to the original Christoffel equation. Numerical examples demonstrate the features of the proposed qS-wave propagators in 2D and 3D TI media. Then we discuss the dynamic features of the pseudo-pure-mode qS-wave equations and the challenges to extending them to anisotropic media with lower symmetry.

**PHASE VELOCITY AND POLARIZATION CHARACTERISTICS**

Following Carcione (2007), we denote the spatial variables \( x, y, \) and \( z \) of a Cartesian system by the indices \( i, j, \ldots = 1, 2, 3 \), respectively, the position vector by \( \mathbf{x} \), a partial derivative with respect to a variable \( x_i \) with \( \partial_i \), and the first and second time derivatives with \( \partial_t \) and \( \partial_{tt} \). Matrix transposition is denoted by the superscript ”\( \top \)”. We also denote the scalar and matrix products by the symbol ”\( \cdot \)”, and the gradient operator by \( \nabla \).

The wave equation in a general heterogeneous anisotropic medium can be expressed as

\[
\rho \partial_{tt} \mathbf{u} = [\nabla C \nabla \top] \mathbf{u} + \mathbf{f},
\]

where \( \mathbf{u} = (u_x, u_y, u_z)\top \) is the particle displacement vector, \( \mathbf{f} = (f_x, f_y, f_z)\top \) represents
the force term, \( \rho \) the density, \( \mathbf{C} \) the matrix representing the stiffness tensor in a two-index notation called the Voigt recipe. The gradient operator has the following matrix representation:

\[
\nabla = \begin{pmatrix}
\partial_x & 0 & 0 & 0 & \partial_z & \partial_y \\
0 & \partial_y & 0 & \partial_z & 0 & \partial_x \\
0 & 0 & \partial_z & \partial_y & \partial_x & 0 \\
\end{pmatrix}.
\] (2)

Neglecting the source term, a plane-wave analysis of the elastic wave equation yields the Christoffel equation,

\[
\tilde{\Gamma} \tilde{\mathbf{u}} = \rho \omega^2 \tilde{\mathbf{u}},
\] (3)

where \( \omega \) is the angular frequency and \( \tilde{\mathbf{u}} = (\tilde{u}_x, \tilde{u}_y, \tilde{u}_z)\top \) is the wavefield in Fourier domain; the wavenumber-domain counterpart of the gradient operator is written as

\[
\tilde{\mathbf{L}} = \begin{pmatrix}
k_x & 0 & 0 & 0 & k_z & k_y \\
0 & k_y & 0 & k_z & 0 & k_x \\
0 & 0 & k_z & k_y & k_x & 0 \\
\end{pmatrix},
\] (4)

in which the propagation direction is specified by the wave vector \( \mathbf{k} = (k_x, k_y, k_z)\top \), and the symmetric Christoffel matrix \( \tilde{\Gamma} = \tilde{\mathbf{L}} \mathbf{C} \tilde{\mathbf{L}}\top \) satisfies:

\[
\tilde{\Gamma} = \begin{pmatrix}
C_{11}k_x^2 + C_{66}k_y^2 + C_{55}k_z^2 & (C_{12} + C_{66})k_xk_y & (C_{13} + C_{55})k_xk_z \\
(C_{12} + C_{66})k_xk_y & C_{66}k_x^2 + C_{22}k_y^2 + C_{44}k_z^2 & (C_{23} + C_{44})k_yk_z \\
(C_{13} + C_{55})k_xk_z & (C_{23} + C_{44})k_yk_z & C_{55}k_x^2 + C_{44}k_y^2 + C_{33}k_z^2 \\
\end{pmatrix}.
\] (5)

The squared phase (or normal) velocities \( V_q^2(q = 1, 2, 3) \) are eigenvalues of the Christoffel matrix. The inequalities

\[
V_1(\mathbf{k}) \geq V_2(\mathbf{k}) \geq V_2(\mathbf{k})
\] (6)

establish the types of waves. Except for anomalous cases of elastic anisotropy, which are of little interest in geophysics, the qP-wave \( (q = 1) \) usually is faster than qS-waves \( (q = 2, 3) \) and the equation

\[
V_1(\mathbf{k}) = V_2(\mathbf{k})
\] (7)

is a great rarity (Yu et al., 1993). However, the equation

\[
V_2(\mathbf{k}) = V_3(\mathbf{k})
\] (8)

is a common event because the phase velocity surfaces (corresponding to qS1 and qS2 waves) can touch or intersect each other (Musgrave, 1970). Directions of wave normals along which the two phase velocities are equal to each other are called acoustic axes or singularity directions. For the shear singularities, the Christoffel matrix is degenerate. Crampin (1991) distinguished three kinds of singularity: point, kiss and line. In point and kiss singularities, the phase velocity surfaces touch at a single point, while in line singularities they intersect. Generally, inserting a nondegenerate eigenvalue back into the Christoffel equation gives ratios of the components of \( \mathbf{u} \), which specify polarization along a given phase direction for a given wave mode. The polarization consists of the
geometrical properties of the particle motion, including trajectory shape and spatial orientation, but excludes magnitudes of the motion. Polarization of an isolated body wave in a noise-free perfectly elastic medium is linear (Winterstein, 1990). In isotropic media, polarizations of such body waves are either parallel to the direction of wave travel, for P-waves, or perpendicular to it, for S-waves. The polarization vectors of the S-wave may take an arbitrary orientation in the plane orthogonal to the P-wave polarization vector. In anisotropic media, however, the polarizations are often neither parallel nor perpendicular to the direction of wave propagation. Whether the medium is anisotropic or not, the polarizations of the three wave modes are always mutually orthogonal for a given propagation direction. So we may separate the elastic wavefield into single-mode scalar fields using the polarization-based projection:

\[ \tilde{\mathbf{w}} = i\mathbf{a}_w \cdot \tilde{\mathbf{u}}, \]

with \( \mathbf{a}_w \) representing the normalized polarization vector of the given mode \( w = \{qP, qS_1, qS_2\} \) (Dellinger, 1991).

In practice, horizontally polarized (or SH) and vertically polarized (or SV) are likely to be the most useful S-wave modes when consideration is restricted to isotropic or TI media, in which all rays lie in symmetry planes. For isotropic media, the above polarization-based projection is material-independent, because the following vectors related to the wave vector \( \mathbf{k} \), i.e.,

\[
\mathbf{e}_1 = \begin{pmatrix} k_x, k_y, k_z \end{pmatrix}^\top, \quad \mathbf{e}_2 = \begin{pmatrix} -k_y, k_x, 0 \end{pmatrix}^\top \quad \text{and} \quad \mathbf{e}_3 = \begin{pmatrix} k_x k_z, k_y k_z, -(k_x^2 + k_y^2) \end{pmatrix}^\top, \tag{10}
\]

indicate the polarization direction of pure P-, SH- and SV-wave, respectively. On the contrary, for anisotropic media, the polarization-based projection depends on local material parameters, because the polarizations are generally specified by the eigenvectors of the original Christoffel equation. For a VTI medium, the stiffness coefficients satisfy: \( C_{12} = C_{11} - 2C_{66}, C_{22} = C_{11}, C_{23} = C_{13} \) and \( C_{55} = C_{44} \). In this case, people still prefer to designate the qS-waves as SH-like and SV-like modes due to the following fact: The use of qS1 and qS2 distinguished by phase velocities does not always give continuous polarization surfaces, while the use of SV and SH distinguished by polarization does, except at the kiss singularity at \( k_x = k_y = 0 \) (Crampin and Yedlin, 1981; Zhang and McMechan, 2010). In this case, the SH-waves polarize perpendicular to the symmetry plane and are pure, and the SV-waves polarize in symmetry planes and are usually quasi-shear. As shown in Figure 1, for both qP and qSV modes, the polarization directions in a VTI material deviate from those in the corresponding isotropic (reference) medium in most propagation directions, but no deviation exists for the SH mode in any direction for either medium. To our interest, the polarization deviations of qP- or qSV-waves between an ordinary VTI medium and its isotropic reference are usually very small, although exceptions are possible (Thomsen, 1986; Tsvankin and Chesnokov, 1990). In addition, taking vectors \( \mathbf{e}_1, \mathbf{e}_2 \) and \( \mathbf{e}_3 \) as the three mutually perpendicular polarization vectors in the unperturbed isotropic medium, approximate formulas for the qP- and qS-wave polarizations in an arbitrary anisotropic medium can be developed using perturbation theory (Cerveny and Jech, 1982; Psencik and Gajewski, 1998; Farra, 2001).
Figure 1: Polarization vectors in a 3D VTI material with $v_{p0} = 3.0 \text{ km/s}$, $v_{s0} = 1.5 \text{ km/s}$, $\epsilon = 0.25$, and $\delta = -0.29$. Its isotropic reference medium is determined by setting $\epsilon = 0$ and $\delta = 0$. One can observe polarization deviations between VTI (red) and its isotropic reference (blue) media for (a) P- and (b) S-waves in most propagation directions, but no deviation for (c) SH-waves in any direction.
To provide for more possibilities and flexibility in describing single-mode wave propagation in anisotropic media, Cheng and Kang (2014) suggest splitting the one-step polarization-based projection into two steps, of which the first step implicitly implements partial wave-mode separation during wavefield extrapolation with a transformed wave equation, while the second step is designed to correct the projection deviation due to the approximation of polarization directions. The transformed wave equation (that they called a pseudo-pure-mode qP-wave equation) was derived from the original Christoffel equation through a similarity transformation aiming to project the displacement wavefield onto the isotropic (reference) polarization direction indicated by $e_1$. In this paper, taking another two orthogonal vectors in equation 10, namely $e_2$ and $e_3$, as the reference polarization directions for SH- and qSV-waves, we apply the same strategy to derive simplified wave equations for these qS-wave modes in general TI media.

**PURE-MODE SH-WAVE EQUATION**

Pure SH-waves horizontally polarize in the planes perpendicular to the symmetry axis of VTI media with $u_z \equiv 0$, so we introduce a similarity transformation to the Christoffel matrix ignoring the vertical component, i.e.,

$$\tilde{\Gamma}_m = M \tilde{\Gamma}_2 M^{-1},$$

with a generally invertible $2 \times 2$ matrix $M$ related to the reference polarization direction $e_2$:

$$M = \begin{pmatrix} -k_y & 0 \\ 0 & k_x \end{pmatrix},$$

and

$$\tilde{\Gamma}_2 = \begin{pmatrix} C_{11} k_x^2 + C_{66} k_y^2 + C_{44} k_z^2 & (C_{12} + C_{66}) k_x k_y \\ (C_{12} + C_{66}) k_x k_y & C_{66} k_x^2 + C_{22} k_y^2 + C_{44} k_z^2 \end{pmatrix}.$$

Accordingly, we derive a transformed Christoffel equation,

$$\tilde{\Gamma}_m \tilde{u} = \rho \omega^2 \tilde{u},$$

for the SH-wave mode:

$$\tilde{u} = M \tilde{u}_2,$$

in which $\tilde{u}_2 = (\tilde{u}_x, \tilde{u}_y)^\top$ represents the horizontal components of the original elastic wavefields, and $\tilde{u} = (\tilde{u}_x, \tilde{u}_y)^\top$ represents the horizontal components of the transformed wavefields. Note that the matrix $M$ will be not invertible when $k_x = 0$ or/and $k_y = 0$. These special directions don’t affect the derivation of the pseudo-pure-mode wave equation for the following reasons: First, we don’t directly project the elastic wavefield into the wavenumber-domain, but instead apply the similarity transformation to the Christoffel equation and eventually inverse the transformed Christoffell equation back into the time-space-domain. Second, the original Christofell matrix $\tilde{\Gamma}_2$ automatically
becomes a diagonal matrix in these directions, so the similarity transformation is not actually needed for the corresponding wavenumber components.

Note the similarity transformation does not change the eigenvalue of the Christoffel matrix corresponding to the SH-wave and, thus, introduces no kinematic error for this wave mode. We also can obtain a kinematically equivalent Christoffel equation if \( M \) is constructed using the normalized form of \( e_2 \) to ensure all spatial frequencies are uniformly scaled. For a locally smooth medium, applying an inverse Fourier transform to equation 14, we obtain a linear second-order system in the time-space domain:

\[
\rho \partial_{tt} \mathbf{u} = \mathbf{\Gamma}_m \mathbf{u},
\]

or in its extended form:

\[
\begin{align*}
\rho \partial_{tt} \overline{u}_x &= C_{11} \partial_{xx} \overline{u}_x + C_{66} \partial_{yy} \overline{u}_x + C_{44} \partial_{zz} \overline{u}_x - (C_{11} - C_{66}) \partial_{yy} \overline{u}_y, \\
\rho \partial_{tt} \overline{u}_y &= C_{66} \partial_{xx} \overline{u}_y + C_{11} \partial_{yy} \overline{u}_y + C_{44} \partial_{zz} \overline{u}_y - (C_{11} - C_{66}) \partial_{xx} \overline{u}_x,
\end{align*}
\]

where \( \overline{u} = (\overline{u}_x, \overline{u}_y)^\top \) represents the horizontal components of SH-wave in time-space domain, and \( \mathbf{\Gamma}_m \) represents the Christoffel differential-operator matrix after the similarity transformation.

Due to the cylindrical symmetry of a TI material, the two equations in equation 17 may be summed to produce a scalar wave equation in terms of \( \overline{u} \):

\[
\rho \partial_{tt} \overline{u} = C_{66} (\partial_{xx} + \partial_{yy}) \overline{u} + C_{44} \partial_{zz} \overline{u},
\]

with \( \overline{u} = \overline{u}_x + \overline{u}_y \) representing the total horizontal components of the transformed SH-wave fields. This is consistent with the fact that only \( C_{44} \) and \( C_{66} \) affect the kinematic signatures of the SH-wave in VTI media (Tsvankin, 2001). In addition, the derived equation naturally reduces to the acoustic wave equation if we apply the isotropic assumption by setting \( C_{44} = C_{66} = \rho V_s^2 \) with \( V_s \) representing the velocity of the isotropic shear wave.

**PSEUDO-PURE-MODE QSV-WAVE EQUATION**

**Derivation of pseudo-pure-mode qSV-wave equation**

For the qSV-wave, we should essentially build a projection from the elastic wavefields \( \widetilde{\mathbf{u}} = (\widetilde{u}_x, \widetilde{u}_y, \widetilde{u}_z)^\top \) to a pseudo-pure-mode wavefield \( \widetilde{\mathbf{u}} = (\widetilde{u}_x, \widetilde{u}_y, \widetilde{u}_z)^\top \). Naturally, we may introduce the following similarity transformation to the Christoffel matrix, i.e.,

\[
\widetilde{\mathbf{\Gamma}}_n = \mathbf{N} \mathbf{\Gamma} \mathbf{N}^{-1},
\]

with the intuitive projection matrix \( \mathbf{N} \) defined by the reference polarization direction \( e_3 \):

\[
\mathbf{N} = \begin{pmatrix}
k_x & 0 & 0 \\
0 & k_y & 0 \\
0 & 0 & -(k_x^2 + k_y^2)
\end{pmatrix},
\]
or its normalized form. However, the resulting pseudo-pure-mode wave equation is very complicated and contains mixed derivatives of time and space. To keep them simple, an intermediate wavefield \( \tilde{\mathbf{u}} = (k_x^2 + k_y^2)\tilde{\mathbf{u}}_z \) is defined by

\[
\tilde{\mathbf{u}}_z = (k_x^2 + k_y^2)\tilde{\mathbf{u}}_z.
\]  

(21)

So we project the vector displacement wavefields using:

\[
\tilde{\mathbf{u}}' = \mathbf{N}'\tilde{\mathbf{u}},
\]  

(22)

with an intermediate projection matrix:

\[
\mathbf{N}' = \begin{pmatrix}
k_xk_x & 0 & 0 \\
0 & k_yk_z & 0 \\
0 & 0 & -1
\end{pmatrix}.
\]  

(23)

Accordingly, we apply the similarity transformation using \( \mathbf{N}' \) to equation (5) and finally get an equivalent Christoffel equation:

\[
\tilde{\Gamma}'_n\tilde{\mathbf{u}}' = \rho\omega^2\tilde{\mathbf{u}}'.
\]  

(24)

with \( \tilde{\Gamma}'_n = \mathbf{N}\bar{\Gamma}(\mathbf{N})^{-1} \).

For a locally smooth medium, applying an inverse Fourier transformation to equation (24), we obtain another coupled forth-order linear system:

\[
\rho\partial_{tt}\mathbf{u}' = \tilde{\Gamma}'_n\mathbf{u}',
\]  

(25)

or in its extended form:

\[
\rho\partial_{tt}\mathbf{u}' = \tilde{\Gamma}'_n\mathbf{u}' = \begin{pmatrix}
\rho\partial_{tt}u_x' \\
\rho\partial_{tt}u_y' \\
\rho\partial_{tt}u_z'
\end{pmatrix}
\]

\[
= (C_{11}\partial_{xx} + C_{66}\partial_{yy} + C_{44}\partial_{zz})u_x + (C_{11} - C_{66})\partial_{xx}u_y + (C_{13} + C_{44})\partial_{xx}\partial_{zz}u_z, \\
\rho\partial_{tt}u_y' = (C_{11} - C_{66})\partial_{yy}u_x + (C_{66}\partial_{xx} + C_{44}\partial_{zz})u_y + (C_{13} + C_{44})\partial_{yy}\partial_{zz}u_z, \\
\rho\partial_{tt}u_z' = (C_{13} + C_{44})\partial_{zz}u_x + (C_{13} + C_{44})\partial_{zz}u_y + C_{44}(\partial_{xx} + \partial_{yy})u_z + C_{33}\partial_{zz}u_z.
\]  

(26)

where \( \mathbf{u}' = (u_x', u_y', u_z')^\top \) is an intermediate wavefield in the time-space domain, and \( \tilde{\Gamma}'_n \) represents the corresponding Christoffel differential-operator matrix after the similarity transformation. The intermediate wavefield has the same horizontal components but a different vertical component of the pseudo-pure-mode wavefield \( \mathbf{u} = (u_x, u_y, u_z)^\top \). Equation (21) indicates that the vertical component satisfies:

\[
\bar{u}_z = -(\partial_{xx} + \partial_{yy})\bar{u}_z.
\]  

(27)

Due to the symmetry property of a VTI material, we may sum the horizontal components and replace the vertical component with the relation given in equation (27).
and finally obtain a simpler second-order system that honors the kinematics of both qP- and qSV-waves:

\[
\rho \frac{\partial^2 u_{xy}}{\partial t^2} = C_{11}(\partial_{xx} + \partial_{yy})u_{xy} + C_{44}\partial_{zz}u_{xy} - (C_{13} + C_{44})\partial_{zz}u_z,
\]

\[
\rho \frac{\partial^2 u_z}{\partial t^2} = -(C_{13} + C_{44})(\partial_{xx} + \partial_{yy})u_{xy} + C_{44}(\partial_{xx} + \partial_{yy})u_z + C_{33}\partial_{zz}u_z,
\]  \(28\)

with \(u_{xy} = u_x + u_y\). Note that pure SH-waves always polarize in the planes perpendicular to the symmetry axis with the polarization direction indicated by \(e_2\), which implies \((k_x k_z)\tilde{u}_x + (k_y k_z)\tilde{u}_y \equiv 0\), i.e., \(\tilde{u}_{xy} \equiv 0\), for the SH-wave. Therefore, the partial summation (after the similarity transformation) automatically removes the SH component from the transformed wavefields. As a result, there are no terms related to \(C_{66}\) any more in equation \(28\). In order to produce a pseudo-pure-mode scalar qSV-wave field, we sum all components of the transformed wavefields, namely

\[
\tilde{u} = \tilde{u}_{xy} + \tilde{u}_z.
\]  \(29\)

For a 2-D VTI medium, equation \(28\) reduces to the following form:

\[
\rho \frac{\partial^2 u_x}{\partial t^2} = C_{11}(\partial_{xx} + \partial_{yy})u_x + C_{44}\partial_{zz}u_x - (C_{13} + C_{44})\partial_{zz}u_z,
\]

\[
\rho \frac{\partial^2 u_z}{\partial t^2} = -(C_{13} + C_{44})(\partial_{xx} + \partial_{yy})u_x + C_{44}(\partial_{xx} + \partial_{yy})u_z + C_{33}\partial_{zz}u_z.
\]  \(30\)

In fact, we can derive the same pseudo-pure-mode wave equation for a 2-D qSV-wave by projecting the 2-D Christoffel matrix onto a reference vector \(e'_3 = (k_z, -k_x)^\top\). Similarly, a 2D pseudo-pure-mode scalar qSV-wave field is given by the summation:

\[
\tilde{u} = \tilde{u}_{xy} + \tilde{u}_z.
\]

If we apply the isotropic assumption by setting \(C_{11} = C_{33}\) and \(C_{13} + C_{44} = C_{33} - C_{44}\), and sum the two equations in equation \(28\) we get the scalar wave equation:

\[
\rho \frac{\partial^2 \tilde{u}}{\partial t^2} = C_{44}(\partial_{xx} + \partial_{yy} + \partial_{zz})\tilde{u},
\]  \(31\)

with \(\tilde{u} = \tilde{u}_{xy} + \tilde{u}_z\) representing a shear wave field, and \(C_{44} = \rho V_s^2\) with \(V_s\) representing the propagation velocity of the isotropic shear wave.

The derived pseudo-pure-mode qSV-wave equations have some interesting and valuable features. First, the projection using matrix \(N\) yields wave-mode separation to some extent, because the chosen projection direction, \(e_3\), represents the polarization direction of the SV-wave in an isotropic medium. As investigated by Tsvankin and Chesnokov (1990) and Psencik and Gajewski (1998), and also demonstrated in Figure 1b, the difference in polarization directions between isotropic and VTI media is generally quite small in most propagation directions for SV-waves. Therefore, considering the mode separator (namely equation \(9\)) and the small projection deviation, summing all the pseudo-pure-mode wavefield components in equation \(28\) or \(30\) partially achieves wave-mode separation and produces a scalar wavefield dominated by the energy of qSV-waves. This will be demonstrated in the numerical examples. Second, the pseudo-pure-mode wave equations are easier to calculate than the original elastic wave equation because they have no terms of mixed partial
derivatives. More importantly, the summation of the horizontal components further simplifies the wave equations and reduces the number of parameters needed for scalar qSV-wave extrapolation. These features are undoubtedly useful for performing multicomponent seismic imaging and inversion that mainly use wavefield kinematics when it is necessary to include anisotropy.

Removing of the residual qP-waves

The pseudo-pure-mode qSV-wave equations are derived by using a similarity transformation that projects the vector displacement wavefield onto the isotropic reference of the qSV-wave’s polarization direction. As demonstrated in Figure 1b, even for a very strong VTI medium, the difference between the two directions is generally quite small in most propagation directions. However, this difference does result in some qP-wave energy remaining in the pseudo-pure-mode scalar qSV-wave fields. To remove the residual qP-waves, we have to correct the projection deviations before summing the pseudo-pure-mode wavefield components. For heterogeneous VTI media, this can be implemented through nonstationary spatial filtering defined by the projection deviations (Cheng and Kang, 2014).

The filters can be constructed once the qSV-wave polarization directions are determined by solving the Christoffel equation based on local medium properties for every grid point. However, this operation is computationally expensive, especially in 3D heterogeneous TI media. We may further reduce the computational cost using a mixed-domain integral algorithm using a low-rank approximation (Cheng and Fomel, 2014). We shall observe in the examples that the residual qP-waves in the pseudo-pure-mode qSV-wave fields are quite weak, even if the anisotropy becomes strong. As explained in Cheng and Kang (2014), it is not necessary to apply the filtering at every time step for many applications, such as RTM.

In the case of transverse isotropy with a tilted symmetry axis (TTI), the elastic tensor loses its simple form and the terminology “in-plane polarization” and “cross-plane polarization” is to be preferred for qSV- and qSH-waves. The generalization of pseudo-pure-mode wave equation to a TTI medium involves no additional physics but greatly complicates the algebra. One strategy for deriving the wave equations is to locally rotate the coordinate system so that its third axis coincides with the symmetry axis; and to make use of the simple form of the wave equation in VTI media (see Cheng and Kang (2014)). Alternatively, we may use some new strategies to derive more numerically stable pseudo-pure-mode wave equations for TTI media with strong variations of parameters (Zhang et al., 2011; Bube et al., 2012). Moreover, the filter to correct the projection deviation can also be constructed with the coordinate rotation.
EXAMPLES

The first example compares the synthetic elastic displacement and pseudo-pure-mode qSV-wave field in 2D homogeneous VTI media with different degrees of anisotropy. Then we demonstrate the computation of 3D synthetic pseudo-pure-mode qSV-wave and pure-mode SH-wave fields for a two-layer VTI model. Finally, we investigate the performance of the pseudo-pure-mode qSV-wave propagator on the 2D BP TTI model. We sue a tenth-order explicit finite-difference scheme on regular grids to solve the involved wave equations. Point sources are located at the centers of the models.

2D homogeneous VTI models

For comparison, we first apply the original elastic wave equation to synthesize wavefields in a homogeneous VTI medium with weak anisotropy, in which \( v_p = 3000 \text{m/s}, \) \( v_s = 1500 \text{m/s}, \) \( \epsilon = 0.1, \) and \( \delta = 0.05. \) Figures 2a and 2b display the horizontal and vertical components of the displacement wavefields at 0.3 s. Then we try to simulate the propagation of a single-mode qSV-wave using the pseudo-pure-mode qSV-wave equation (namely equation [30]). Figure 2c and 2d display the two components of the pseudo-pure-mode qSV-wave fields, and Figure 2e displays their summation, i.e., the pseudo-pure-mode scalar qSV-wave fields with weak residual qP-wave energy. We observe that, in most propagation directions, the polarities are almost reversed for the wavefronts of qP-waves in the two components of the pseudo-pure-mode qSV-wave fields. This contributes to suppressing the qP-wave energy through summation of the two components. Compared with the theoretical wavefront curves (see Figure 2f) calculated using group velocities and angles, pseudo-pure-mode scalar qSV-wave fields have correct kinematics for both qP- and qSV-waves. We finally remove residual qP-waves by applying the filtering to correct the projection deviation and get completely separated scalar qSV-wave fields (Figure 2g).

Next, we consider wavefield modeling in a homogeneous VTI medium with strong anisotropy, in which \( v_p = 3000 \text{m/s}, v_s = 1500 \text{m/s}, \) \( \epsilon = 0.25, \) and \( \delta = -0.25. \) Figure 3 displays the wavefield snapshots at 0.3 s synthesized both by using the original elastic wave equation and the pseudo-pure-mode qSV-wave equation. Note that the pseudo-pure-mode qSV-wave equation still accurately represents the qP- and qSV-waves’ kinematics. Although the residual qP-wave energy becomes stronger when the degree of anisotropy increases, the filtering step still removes them effectively. It takes CPU times of 0.15 and 0.06 seconds to extrapolate the elastic and pseudo-pure-mode qSV-wave fields for one time-step, respectively. But it takes about 8.2 seconds to remove the residual qP-wave from the pseudo-pure-mode qSV-wave fields using wavenumber-domain filtering. In fact, separating the pure-mode wavefield from the elastic and pseudo-pure-mode wavefields has almost the same computational cost for TI media (Cheng and Kang, 2014).
Figure 2: Synthesized wavefields in a VTI medium with weak anisotropy: (a) x- and (b) z-components synthesized by original elastic wave equation; (c) x- and (d) z-components synthesized by pseudo-pure-mode qSV-wave equation; (e) pseudo-pure-mode scalar qSV-wave fields; (f) kinematics of qV- and qSV-waves and (g) separated scalar qSV-wave fields.

Figure 3: The same plots as Figure 2 but for a VTI medium with stronger anisotropy.
3D two-layer VTI model

Figure 4 shows an example of simulating the propagation of pseudo-pure-mode qSV-wave fields in a 3D two-layer VTI model (see Figure 4a), with \( v_{p0} = 2500 \text{m/s} \), \( v_{s0} = 1200 \text{m/s} \), \( \epsilon = 0.25 \), \( \delta = -0.25 \) and \( \gamma = 0.3 \) in the first layer, and \( v_{p0} = 3600 \text{m/s} \), \( v_{s0} = 1800 \text{m/s} \), \( \epsilon = 0.2 \), \( \delta = 0.1 \) and \( \gamma = 0.05 \) in the second layer. We propagate the 3D pseudo-pure-mode qSV-wave fields using equation 28. Figure 4d displays the pseudo-pure-mode scalar qSV-wave fields resulting from the summation of the horizontal (Figure 4b) and vertical (Figure 4c) components, namely \( \pi_{xy} \) and \( \pi_z \). We see that the qS-waves dominate the scalar wavefields in energy. As shown in Figure 5, we also obtain pure-mode scalar SH-wave fields either using the summation of the horizontal components synthesized by using the pseudo-pure-mode wave equation 17 or directly using the scalar wave equation, i.e., equation 18.

BP 2007 TTI model

Finally, we demonstrate pseudo-pure-mode qSV-wave propagation in the 2D BP TTI model (see Figure 6). The space grid size is 12.5 m and the time step is 1 ms for high-order finite-difference operators. Here the vertical velocities for the qSV-wave are set to half of the qP-wave velocities. Figure 7 displays snapshots of wavefield components at the time of 1.4s synthesized by using the original elastic wave equation and the pseudo-pure-mode qSV-wave equation. In the elastic wavefields, we observe strong scattered and mode-converted energy in the region with a rapidly varying anisotropic symmetry axis direction. For comparison, in Figures 7c and 7d, we also show the separated qP- and qSV-wave scalar fields obtained using the approach proposed by Cheng and Fomel (2014). Not that in the pseudo-pure-mode qSV-wave fields (see Figure 7g), the incident qP-waves as well as scattered and converted qP-waves are effectively suppressed. The spatial filtering appears to remove residual qP-waves and accurately separates qSV-wave data (including the converted qP-qSV waves) from the pseudo-pure-mode wavefields in this complex model (Figure 7h). Vertical slices through the scalar fields (Figure 8) provide further proof to evaluate the performance of the proposed qS-wave propagators. As we observed, in heterogeneous rough zones with strong variations in tilt angle, there are differences between the elastic and pseudo-pure-mode qSV-wave fields. Fortunately, the pseudo-pure-mode qSV-wave equation still captures the shear wave kinematics to a great extent. For a single time-step, it respectively takes CPU times of 2.71 and 1.22 seconds to extrapolate the elastic and pseudo-pure-mode qSV-wave fields, and about 7.50 seconds to separate the qSV-wave fields from both wavefields using low-rank approximate mixed-domain integral operations based on the qSV-wave’s polarization directions (Cheng and Fomel, 2014).
Figure 4: Synthesized wavefield snapshots in a 3D two-layer VTI model using equation [28]: (a) vertical velocity of qSV-wave, (b) horizontal component $u_{xy}$ and (c) vertical component $u_z$ of the pseudo-pure-mode qSV-wave fields, (d) pseudo-pure-mode scalar qSV-wave fields. The dash line indicates the interface.
Figure 5: Synthesized wavefield snapshots in a 3D two-layer VTI model using equation 17: (a) x- and (b) y-components of the pseudo-pure-mode wavefields, (c) pure-mode scalar SH-wave fields calculated as the summation of the two horizontal components of the pseudo-pure-mode wavefields. Note that the same scalar wavefields are obtained if we directly use the scalar wave equation for SH-waves, namely equation 18.

[qswave/twolayer3dvti/ SHxInterf,SHyInterf,SHInterf]
Figure 6: Partial region of the 2D BP TTI model: (a) vertical qP-wave velocity, Thomsen coefficients (b) $\epsilon$ and (c) $\delta$, and (d) the tilt angle $\theta$.

DISCUSSION

Kinematic and dynamic accuracy

The similarity transformation to the Christoffel equation preserves the kinematics of the qS-waves, but inevitably change the phases and amplitudes in their wavefields. Accordingly, the pseudo-pure-mode wave equations may change the radiation from a point source (as demonstrated in the examples), and even distort the amplitude variation with offset (AVO). In other word, they do not honor the dynamic elasticity of the waves in real media. In fact, other simplified forms of the elastic wave equation, such as acoustic or pseudo-acoustic wave equations and the pure-mode approximate wave equations, have similar limitations (Barnes and Charara, 2009, Operto et al., 2009, Cheng and Kang, 2014, Shang et al., 2015). For heterogeneous rough media, i.e., when scales for variations in the elastic parameters are small compared with the wavelengths of the wavefield, the acoustic approximation is no longer reliable (Cance and Capdeville, 2015). The pseudo-pure-mode wave equations have similar limitations for shear-wave modeling in high-contrast TI media. However, these limitations are not doomed to be catastrophic, because velocity models containing high-wavenumber components are rarely involved at most stages of seismic imaging and inversion for real data.
Figure 7: Synthesized wavefield snapshots on BP 2007 TTI model using original elastic wave equation and pseudo-pure-mode qSV-wave equation respectively: (a) x- and (b) z-components synthesized by elastic wave equation; (c) scalar qP- and (d) scalar qSV-wave fields separated from the elastic wavefield; (e) x- and (f) z-components synthesized by pseudo-pure-mode qSV-wave equation; (g) pseudo-pure-mode scalar qSV-wave field and (h) pure-mode scalar qSV-wave field separated from the pseudo-pure-mode qSV-wave field.
Propagate separated qS-wave modes

Figure 8: Vertical slices through the scalar wavefields at \( x = 50.5 \) km in Figure 7: (a) qSV-wave separated from the elastic wavefield; (b) pseudo-pure-mode qSV-wave; (c) pure qSV-wave separated from the pseudo-pure-mode wavefield.

Challenge for anisotropy with lower symmetry

Unlike the well-behaved qP-wave mode, the qS-wave modes do not consistently polarize as a function of propagation direction, and thus cannot be designated as SV- and SH-waves, except in isotropic and TI media [Winterstein, 1990]. To demonstrate the difficulties of extending the methodology in this paper to anisotropic media with symmetry lower than TI, we first compare the polarization features of qS-waves in typical TI and orthorhombic anisotropic rocks. Figure 9 shows polarizations of qS1- and qS2-waves in a VTI material - Mesaverde shale [Thomsen, 1986], which has the parameters \( v_p^0 = 3.749 \) km/s, \( v_s^0 = 2.621 \) km/s, \( \epsilon = 0.225 \), \( \delta = 0.078 \), and \( \gamma = 0.100 \). The polarization directions are either horizontal or vertical (in the symmetry plane), so that we can definitely designate qS-waves as qSV- and SH-wave modes, except at the kiss singularity. Figure 10 shows polarizations of qS1- and qS2-waves in a “standard” orthorhombic anisotropic material - vertically fractured shale [Schoenberg and Helbig, 1997], which has the parameters \( v_p^0 = 2.437 \), \( v_s^0 = 1.265 \) km/s, \( \epsilon_1 = 0.329 \), \( \epsilon_2 = 0.258 \), \( \delta_1 = 0.083 \), \( \delta_2 = -0.078 \), \( \delta_3 = -0.106 \), \( \gamma_1 = 0.182 \) and \( \gamma_2 = 0.0455 \). The qS-waves polarize in a very complicated way and have point singularities in many propagation directions.

Shear-wave modeling is complicated by the presence of the shear-wave singularities. As investigated by [Crampin and Yedlin, 1981], a TI material only has line and kiss singularities, while other anisotropic materials excluding those with triclinic symmetry (e.g., orthorhombic and monoclinic anisotropic materials) have point singularities in many propagation directions. Line singularities occur only at a fixed
angle from the symmetry axis and cause no distortion of phase velocity surfaces or polarization phenomena. For kiss singularities (along the direction of symmetry axis), qS-wave polarizations vary rapidly in their vicinity but are well-behaved because there is no distortion in phase-velocity surfaces. These features facilitate the derivations of pseudo-pure-mode qSV-wave and pure-mode SH-wave equations for TI media. For directions near point singularities, however, the polarization of plane qS-waves changes very rapidly, and amplitudes and polarizations of qS-waves with curved wavefronts behave quite anomalously. Therefore, although pseudo-pure-mode qP-wave equations exist for general anisotropic media, it may be more confusing than helpful to extend the proposed pseudo-pure-mode qS-wave equations to symmetry systems lower than TI.

Figure 9: Polarization vectors of 3D qS-waves in a VTI material (Mesaverde shale): (a) qS1-wave; (b) qS2-wave.
Figure 10: Polarization vectors of 3D qS-waves in an orthorhombic anisotropic material: (a) qS1-wave; (b) qS2-wave.
CONCLUSIONS

By applying two different similarity transformations to the original Christoffel equation, which aim to project the vector displacement wavefields onto the isotropic SV- and SH-waves’ polarization directions, we have derived the pseudo-pure-mode qSV-wave equation and the pure-mode SH-wave equation for 2D and 3D heterogeneous TI media, respectively. These equations are simpler than the original elastic wave equation and involve less material parameters, which reduces computational cost at least by half if the finite-difference scheme is used in practice. The theoretical analysis and numerical examples have demonstrated that, the pseudo-pure-mode qS-wave propagators for TI media have the following features: First, the qSV-wave equations honor the kinematics for both qP and qSV modes, while the pure-mode SH-wave equation guarantees the kinematics for the scalar SH-wave. Second, although qP-waves still remain in the pseudo-pure-mode qSV-wave fields, their horizontal and vertical components have almost opposite polarities in most propagation directions. As a result, the summation of all components produces a pseudo-pure-mode scalar qSV-wave field with very weak qP-wave energy. Third, the non-SH parts in the pseudo-pure-mode vector SH-wave field have completely opposite polarities, and thus are thoroughly removed from the scalar SH-wave field once all components are summed. In addition, a filtering step taking into account the polarization deviation can be used to thoroughly remove the residual qP-waves for pseudo-pure-mode scalar qSV-wave extrapolation. These features indicate the potential of the proposed qS-wave propagators for developing promising seismic imaging and inversion algorithms in heterogeneous TI media. Like the pseudo-acoustic or pseudo-pure-mode qP-wave equations, the proposed pseudo-pure-mode qS-wave equations take into account “scalar anisotropy” and may distort the dynamic elasticity of the real anisotropic media.

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REFERENCES

Propagate separated qS-wave modes


Farra, V., 2001, High-order perturbations of the phase velocity and polarization of
qp and qs waves in anisotropic media: Geophysical Journal International, 147, 93–104.
Hardage, B. A., M. V. DeAngelo, P. E. Murray, and D. Sava, 2011, Multicomponent seismic technology: SEG.
Li, X. Y., 1997, Fractured reservoir delineation using multicomponent seismic data: Geophysical Prospecting, 45, 39–64.
———, 1999, C-wave reflection seismology over inhomogeneous and anisotropic media: Geophysics, 64, 678–690.


Simulating propagation of separated wave modes in general anisotropic media, Part I: qP-wave propagators

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ABSTRACT

Wave propagation in an anisotropic medium is inherently described by elastic wave equations, with P- and S-wave modes intrinsically coupled. We present an approach to simulate propagation of separated wave modes for forward modeling, migration, waveform inversion and other applications in general anisotropic media. The proposed approach consists of two cascaded computational steps. First, we simulate equivalent elastic anisotropic wavefields with a minimal second-order coupled system (that we call here a pseudo-pure-mode wave equation), which describes propagation of all wave modes with a partial wave mode separation. Such a system for qP-wave is derived from the inverse Fourier transform of the Christoffel equation after a similarity transformation, which aims to project the original vector displacement wavefields onto isotropic references of the polarization directions of qP-waves. It accurately describes the kinematics of all wave modes and enhances qP-waves when the pseudo-pure-mode wavefield components are summed. The second step is a filtering to further project the pseudo-pure-mode wavefields onto the polarization directions of qP-waves so that residual qS-wave energy is removed and scalar qP-wave fields are accurately separated at each time step during wavefield extrapolation. As demonstrated in the numerical examples, pseudo-pure-mode wave equation plus correction of projection deviation provides a robust and flexible tool for simulating propagation of separated wave modes in transversely isotropic and orthorhombic media. The synthetic example of Hess VTI model shows that the pseudo-pure-mode qP-wave equation can be used in prestack reverse-time migration (RTM) applications.

INTRODUCTION

All anisotropy arises from ordered heterogeneity much smaller than the wavelength [Winterstein 1990]. With the increased resolution of seismic data and because of wider seismic acquisition aperture (both with respect to offset and azimuth), there is a growing awareness that an isotropic description of the Earth may no longer be adequate. Anisotropy appears to be a near-ubiquitous property of earth materials, and its effects on seismic data must be quantified.
Wave equation is the central ingredient in characterizing wave propagation for seismic imaging and elastic parameters inversion. In isotropic media, it is common to use scalar acoustic wave equations to describe the propagation of seismic data as representing only P-wave energy (Yilmaz, 2001). Compared to the elastic wave equation, the acoustic wave equation is simpler and more efficient to use, and does not yield S-waves for modeling of P-waves. Anisotropic media are inherently described by elastic wave equations with P- and S-wave modes intrinsically coupled. It is well known that a S-wave passing through an anisotropic medium splits into two mutually orthogonal waves (Crampin, 1984). Generally the P-wave and the two S-waves are not polarized parallel and perpendicular to the wave vector, thus are called quasi-P (qP) and quasi-S (qS) waves. However, most anisotropic migration implementations do not use the full elastic anisotropic wave equation because of the high computational cost involved, and the difficulties in separating wavefields into different wave modes. Although an acoustic wave does not exist in anisotropic media, Alkhalifah (2000) introduced a pseudo-acoustic approximate dispersion relation for vertically transverse isotropic (VTI) media by setting the shear velocity along the axis of symmetry to zero, which leads to a fourth-order partial differential equation (PDE) in space-time domain. Following the same procedure, he also presented a pseudo-acoustic wave equation of sixth-order in vertical orthorhombic (ORT) anisotropic media (Alkhalifah, 2003). Many authors have implemented pseudo-acoustic VTI modeling and migration based on various coupled second-order PDE systems derived from Alkhalifah’s dispersion relation (Alkhalifah, 2000; Klie and Toro, 2001; Zhou et al., 2006b; Hestholm, 2007). Alternatively, coupled first-order and second-order systems are derived starting from first principles (the equations of motion and Hooke’s law) under the pseudo-acoustic approximation for VTI media (Duveneck and Bakker, 2011) and recently for orthorhombic media as well (Fowler and King, 2011; Zhang and Zhang, 2011). The pseudo-acoustic tilted transversely isotropic (TTI) or tilted orthorhombic wave equations can be obtained from their pseudo-acoustic VTI (or pseudo-acoustic vertical orthorhombic) counterparts by simply performing a coordinate rotation according to the directions of the symmetry axes (Zhou et al., 2006a; Fletcher et al., 2009). Pseudo-acoustic wave equations have been widely used for RTM in transversely isotropic (TI) media because they describe the kinematic signatures of qP-waves with sufficient accuracy and are simpler than their elastic counterparts, which leads to computational savings in practice.

On the other hand, the pseudo-acoustic approximation may result in some problems in characterizing wave propagation in anisotropic media. First, to enhance computational stability, pseudo-acoustic approximations reduce the freedom to choose the material parameters compared with their elastic counterparts (Grechka et al., 2004). Practitioners often observe instability in practice when the pseudo-acoustic equations are used in complex TI media (Fletcher et al., 2009; Zhang et al., 2011; Bube et al., 2012). Stable RTM implementations in TTI media can be achieved by using pseudo-acoustic wave equations derived directly from first principles (Duveneck and Bakker, 2011) using self-adjoint or covariant derivative operators (Macesanu, 2011; Zhang et al., 2011). Second, the widely-used pseudo-acoustic approximation still results in
significant shear wave presence in both modeling data and RTM images (Zhang et al., 2003; Grechka et al., 2004; Jin et al., 2011). It is not easy to get rid of qSV-waves from the wavefields simulated by the pseudo-acoustic wave equations when a full waveform modeling for qP-wave is required. Placing both sources and receivers into an artificial isotropic or elliptic anisotropic acoustic layer could eliminate many of the undesired qSV-wave energy (Alkhalifah, 2000), but the propagated qP-wave may get converted to qSV-wave and the qSV-wave might get converted back to qP-wave in other portions of the model. A projection filtering based on an approximate representation of characteristic-waveform of qP-waves was suggested to suppress undesired qSV-wave energy at each output time step (Zhang et al., 2009). But qS-wave artifacts still remain and qP-wave amplitudes may be not correctly restored due to the approximation introduced in the used wave equation. To avoid the qSV-wave energy completely, different approaches have recently been proposed to model the pure qP-wave propagation in VTI and TTI media. The optimized separable approximation (Liu et al., 2009; Zhang and Zhang, 2009; Du et al., 2010), the pseudo-analytical method (Etgen and Brandsberg-Dahl, 2009), the low-rank approximation (Fomel et al., 2013), the Fourier finite-difference method (Song and Fomel, 2011) and the rapid expansion method (Pestana and Stoffa, 2010) belong to this category.

In fact, anisotropic phenomena are especially noticeable in shear and mode-converted wavefields. Therefore, modeling of anisotropic shear waves may be important both on theoretical and practical aspects. Liu et al. (2009) factorized the pseudo-acoustic VTI dispersion relation and obtained two pseudo-partial differential (PPD) equations, of which the qP-wave equation is well-posed for any value of the anisotropic parameters, but the qSV-wave equation becomes well-posed only when the condition \( \epsilon > \delta \) is satisfied. These PPD equations are very hard to solve in heterogeneous media unless further approximations are introduced (Liu et al., 2009; Chu et al., 2011) or recently developed FFT-based approaches are used (Pestana et al., 2011; Song and Fomel, 2011; Fomel et al., 2013). Note that some of the above efforts to model pure-mode wavefields suffer from accuracy loss more or less due to the approximations to the phase velocities or dispersion relations. Furthermore, these pure-mode propagators only consider the phase term in wave propagation, so they are appropriate for seismic migration but not necessarily for accurate seismic modeling, which may require taking account of amplitude effects and other elastic phenomena such as mode conversion.

In kinematics, there are various forms equivalent to the original first- or second-order elastic wave equations. Mathematically, analysis of the dispersion relation as matrix eigenvalue system allows one to generate equivalent coupled linear second-order systems by similarity transformations (Fowler et al., 2010). Accordingly, Kang and Cheng (2011) proposed new coupled second-order systems for both qP- and qS-waves in TI media by applying specified similarity transformations to the Christoffel equation. Their coupled system for qP-waves represents dominantly the energy propagation of scalar qP-waves while that for qSV-waves propagates dominantly the scalar qSV-wave energy. However, each of the two systems still contains relatively weak residual energy of the other mode. Cheng and Kang (2012) and Kang and Cheng (2012) called such coupled systems “pseudo-pure-mode wave equations” and further
proposed an approach to get separated qP- or qS-wave data from the pseudo-pure-
mode wavefields in general anisotropic media. In the two articles of this series, we
demonstrate how to simulate propagation of separated wave-modes based on a new
simplified description of wave propagation in general anisotropic media. We shall
focus on qP- and qS-waves in each article separately.

The first paper is structured as follows: First, we revisit the plane-wave analysis
of the full elastic anisotropic wave equation. Then we introduce a similarity transfor-
mation to the Christoffel equation required to derive the pseudo-pure-mode qP-wave
equation, and give the simplified forms under pseudo-acoustic or/and isotropic ap-
proximations to illustrate the physical interpretation. After that, we discuss how to
obtain separated qP-wave data from the extrapolated wavefields coupled with resid-
ual qS-waves. Finally, we show numerical examples to demonstrate the features and
advantages of our approach in wavefield modeling and RTM in TI and orthorhombic
media.

PSEUDO-PURE-MODE COUPLED SYSTEM FOR
QP-WAVES

Plane-wave analysis of the elastic wave equation

Vector and component notations are used alternatively throughout the paper. The
wave equation in general heterogeneous anisotropic media can be expressed as (Car-
cione, 2001),

\[ \rho \frac{\partial^2 u}{\partial t^2} = [\nabla \mathbf{C} \nabla^T] \mathbf{u} + \mathbf{f}, \]

where \( \mathbf{u} = (u_x, u_y, u_z)^T \) is the particle displacement vector, \( \mathbf{f} = (f_x, f_y, f_z)^T \) represents
the force term, \( \rho \) is the density, \( \mathbf{C} \) is the matrix representing the stiffness tensor in a
two-index notation called the Voigt recipe, and the symmetric gradient operator has
the following matrix representation:

\[ \nabla = \begin{pmatrix} \frac{\partial}{\partial x} & 0 & 0 & \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ 0 & 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{pmatrix}. \]

Assuming that the material properties vary sufficiently slowly so that spatial deriv-
atives of the stiffnesses can be ignored, equation 1 can be simplified as

\[ \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \Gamma \mathbf{u} + \mathbf{f}, \]
where $\Gamma$ is the $3 \times 3$ symmetric Christoffel differential-operator matrix, of which the elements are given for locally smooth media as follows (Auld, 1973),

$$
\begin{align*}
\Gamma_{11} &= C_{11} \frac{\partial^2}{\partial x^2} + C_{66} \frac{\partial^2}{\partial y^2} + C_{55} \frac{\partial^2}{\partial z^2} + 2C_{56} \frac{\partial^2}{\partial y \partial z} + 2C_{15} \frac{\partial^2}{\partial x \partial z} + 2C_{16} \frac{\partial^2}{\partial x \partial y}, \\
\Gamma_{22} &= C_{66} \frac{\partial^2}{\partial x^2} + C_{22} \frac{\partial^2}{\partial y^2} + C_{44} \frac{\partial^2}{\partial z^2} + 2C_{24} \frac{\partial^2}{\partial y \partial z} + 2C_{46} \frac{\partial^2}{\partial x \partial z} + 2C_{26} \frac{\partial^2}{\partial x \partial y}, \\
\Gamma_{33} &= C_{55} \frac{\partial^2}{\partial x^2} + C_{44} \frac{\partial^2}{\partial y^2} + C_{33} \frac{\partial^2}{\partial z^2} + 2C_{34} \frac{\partial^2}{\partial y \partial z} + 2C_{35} \frac{\partial^2}{\partial x \partial z} + 2C_{45} \frac{\partial^2}{\partial x \partial y}, \\
\Gamma_{23} &= C_{56} \frac{\partial^2}{\partial x^2} + C_{24} \frac{\partial^2}{\partial y^2} + C_{34} \frac{\partial^2}{\partial z^2} + (C_{44} + C_{23}) \frac{\partial^2}{\partial y \partial z} + (C_{36} + C_{45}) \frac{\partial^2}{\partial x \partial z} \\
&+ (C_{25} + C_{46}) \frac{\partial^2}{\partial x \partial y}, \\
\Gamma_{13} &= C_{15} \frac{\partial^2}{\partial x^2} + C_{46} \frac{\partial^2}{\partial y^2} + C_{35} \frac{\partial^2}{\partial z^2} + (C_{45} + C_{36}) \frac{\partial^2}{\partial y \partial z} + (C_{13} + C_{55}) \frac{\partial^2}{\partial x \partial z} \\
&+ (C_{14} + C_{56}) \frac{\partial^2}{\partial x \partial y}, \\
\Gamma_{12} &= C_{16} \frac{\partial^2}{\partial x^2} + C_{26} \frac{\partial^2}{\partial y^2} + C_{45} \frac{\partial^2}{\partial z^2} + (C_{46} + C_{25}) \frac{\partial^2}{\partial y \partial z} + (C_{14} + C_{56}) \frac{\partial^2}{\partial x \partial z} \\
&+ (C_{12} + C_{66}) \frac{\partial^2}{\partial x \partial y}.
\end{align*}
$$

For the most important types of seismic anisotropy such as transverse isotropy and orthorhombic anisotropy, some terms in equation 4 vanish because the corresponding stiffness coefficients become zeros.

Neglecting the source term, a plane-wave analysis of the elastic anisotropic wave equation yields the Christoffel equation,

$$
\tilde{\Gamma} \tilde{u} = \rho \omega^2 \tilde{u},
$$

or

$$
(\tilde{\Gamma} - \rho \omega^2 \mathbf{I}) \tilde{u} = \mathbf{0},
$$

where $\omega$ is the frequency, $\tilde{u} = (\tilde{u}_x, \tilde{u}_y, \tilde{u}_z)^T$ is the wavefield in Fourier domain, $\tilde{\Gamma} = \tilde{\mathbf{L}} \mathbf{C} \tilde{\mathbf{L}}^T$ is the symmetric Christoffel matrix, $\mathbf{I}$ is a $3 \times 3$ identity matrix. To support the sign notation in equations 5 and 6 we remove the imaginary unit $i$ of the wavenumber-domain counterpart of the gradient operator $\nabla$ and thus express matrix $\tilde{\mathbf{L}}$ as:

$$
\tilde{\mathbf{L}} = \begin{pmatrix} k_x & 0 & 0 & 0 & k_z & k_y \\
0 & k_y & 0 & k_z & 0 & k_x \\
0 & 0 & k_x & k_y & k_z & 0 \end{pmatrix}.
$$

Setting the determinant of $\tilde{\Gamma} - \rho \omega^2 \mathbf{I}$ in equation 6 to zero gives the characteristic equation, and expanding that determinant gives the (angular) dispersion relation.
For a given spatial direction specified by a wave vector \( \mathbf{k} = (k_x, k_y, k_z)^T \), the characteristic equation poses a standard 3 \times 3 eigenvalue problem. The three eigenvalues correspond to the phase velocities of the qP-wave and two qS waves. Inserting one of the eigenvalues back into the Christoffel equation gives ratios of the components of \( \tilde{\mathbf{u}} \), from which the polarization or displacement direction can be determined for the given wave mode. In general, these directions are neither parallel nor perpendicular to the wave vector, and depend on the local material parameters for the anisotropic medium. For a given wave vector or slowness direction, the polarization vectors of the three wave modes are always mutually orthogonal.

Applying an inverse Fourier transform to the dispersion relation yields a high-order PDE in time and space and contains mixed space and time derivatives. Setting the shear velocity along the axis of symmetry to zero while using Thomsen’s parameter notation yields the pseudo-acoustic dispersion relation and wave equation in VTI media (Alkhalifah 2000). Most published methods instead have used coupled PDEs (derived from the pseudo-acoustic dispersion relation) that are only second-order in time and eliminate the mixed space-time derivatives, e.g., Zhou et al. (2006b). Many kinematically equivalent coupled second-order systems can be generated from the dispersion relation by similarity transformations (Fowler et al., 2010). In the next section, we present a particular similarity transformation to the Christoffel equation in order to derive a minimal second-order coupled system, which is helpful for simulating propagation of separated qP-waves in anisotropic media.

**Pseudo-pure-mode qP-wave equation**

To describe propagation of separated qP-waves in anisotropic media, we first revisit the classical wave mode separation theory. In isotropic media, scalar P-wave can be separated from the extrapolated vector wavefield \( \mathbf{u} \) by applying a divergence operation: \( P = \nabla \cdot \mathbf{u} \). In the wavenumber domain, this can be equivalently expressed as a dot product that essentially projects the wavefield \( \tilde{\mathbf{u}} \) onto the wave vector \( \mathbf{k} \), i.e.,

\[
\tilde{P} = i\mathbf{k} \cdot \tilde{\mathbf{u}},
\]  

Similarly, for an anisotropic medium, scalar qP-waves can be separated by projecting the vector wavefields onto the true polarization directions of qP-waves by (Dellinger and Etgen, 1990),

\[
q\tilde{P} = i\mathbf{a}_p \cdot \tilde{\mathbf{u}},
\]  

where \( \mathbf{a}_p = (a_{px}, a_{py}, a_{pz})^T \) represents the polarization vector for qP-waves. For heterogeneous models, this scalar projection can be performed using nonstationary spatial filtering depending on local material parameters (Yan and Sava, 2009).

To provide more flexibility for characterizing wave propagation in anisotropic media, we suggest to split the one-step projection into two steps, of which the first step implicitly implements partail wave mode separation (like in equation (8)) during wavefield extrapolation with a transformed wave equation, while the second step is
designed to correct the projection deviation implied by equations 8 and 9. We achieve this on the base of the following observations: the difference of the polarization between an ordinary anisotropic medium and its isotropic reference at a given wave vector direction is usually small, though exceptions are possible (Thomsen, 1986; Tsvankin and Chesnokov, 1990); The wave vector can be taken as the isotropic reference of the polarization vector for qP-waves; It is a material-independent operation to project the elastic wavefield onto the wave vector.

Therefore, we introduce a similarity transformation to the Christoffel matrix, i.e.,

\[ \tilde{\Gamma} = M_p \tilde{\gamma} M_p^{-1}, \]

with a invertible \(3 \times 3\) matrix \(M_p\) related to the wave vector:

\[ M_p = \begin{pmatrix} ik_x & 0 & 0 \\ 0 & ik_y & 0 \\ 0 & 0 & ik_z \end{pmatrix}. \]

Accordingly, we derive an equivalent Christoffel equation,

\[ \tilde{\Gamma} \tilde{u} = \rho \omega^2 \tilde{u}, \]

for a transformed wavefield:

\[ \tilde{u} = M_p \tilde{u}. \]

The above similarity transformation does not change the eigenvalues of the Christoffel matrix and thus introduces no kinematic errors for the wavefields. By the way, we can obtain the same transformed Christoffel equation if matrix \(M_p\) is constructed using the normalized wavenumbers to ensure all spatial frequencies are uniformly scaled. For a locally smooth medium, applying an inverse Fourier transform to equation 12, we obtain a coupled linear second-order system kinematically equivalent to the original elastic wave equation:

\[ \rho \frac{\partial^2 \tilde{u}}{\partial t^2} = \tilde{\Gamma} \tilde{u}, \]

where \(\tilde{u}\) represents the time-space domain wavefields, and \(\tilde{\Gamma}\) represents the Christoffel differential-operator matrix after the similarity transformation.

For the transformed elastic wavefield in the wavenumber-domain, we have

\[ \tilde{u} = \tilde{u}_x + \tilde{u}_y + \tilde{u}_z = i \mathbf{k} \cdot \tilde{u}. \]

And in space-domain, we also have

\[ \tilde{u} = u_x + u_y + u_z = \nabla \cdot \mathbf{u}, \]

with

\[ u_x = \frac{\partial u_x}{\partial x}, \quad u_y = \frac{\partial u_y}{\partial y}, \quad \text{and} \quad u_z = \frac{\partial u_z}{\partial z}. \]
These imply that the new wavefield components essentially represent the spatial derivatives of the original components of the displacement wavefield, and the transformation (equation [13]) plus the summation of the transformed wavefield components (like in equation [15] or [16]) essentially finishes a scalar projection of the displacement wavefield onto the wave vector. For isotropic media, such a projection directly produces scalar P-wave data. In an anisotropic medium, however, only a partial wave-mode separation is achieved because there is usually a direction deviation between the wave vector and the polarization vector of qP-wave. Generally, this deviation turns out to be small and its maximum value rarely exceeds 20° for typical anisotropic earth media (Psencik and Gajewski, 1998). Because of the orthogonality of qP- and qS-wave polarizations, the projection deviations of qP-waves are generally far less than those of the qSV-waves when the elastic wavefields are projected onto the isotropic references of the qP-wave’s polarization vectors. As demonstrated in the synthetic examples of various symmetry and strength of anisotropy, the scalar wavefield \( \pi \) represents dominantly the energy of qP-waves but contains some weak residual qS-waves. This is why we call the coupled system (equation [14]) a pseudo-pure-mode wave equation for qP-wave in anisotropic media.

Substituting the corresponding stiffness matrix into the above derivations, we get the extended expression of pseudo-pure-mode qP-wave equation for any anisotropic media. As demonstrated in Appendix A, pseudo-pure-mode qP-wave equation in vertical TI and orthorhombic media can be expressed as

\[
\begin{align*}
\rho \frac{\partial^2 \pi_x}{\partial t^2} &= C_{11} \frac{\partial^2 \pi_x}{\partial x^2} + C_{66} \frac{\partial^2 \pi_x}{\partial y^2} + C_{55} \frac{\partial^2 \pi_x}{\partial z^2} + (C_{12} + C_{66}) \frac{\partial^2 \pi_y}{\partial x^2} + (C_{13} + C_{55}) \frac{\partial^2 \pi_z}{\partial x^2}, \\
\rho \frac{\partial^2 \pi_y}{\partial t^2} &= C_{66} \frac{\partial^2 \pi_y}{\partial x^2} + C_{22} \frac{\partial^2 \pi_y}{\partial y^2} + C_{44} \frac{\partial^2 \pi_y}{\partial z^2} + (C_{12} + C_{66}) \frac{\partial^2 \pi_z}{\partial y^2} + (C_{23} + C_{44}) \frac{\partial^2 \pi_z}{\partial y^2}, \\
\rho \frac{\partial^2 \pi_z}{\partial t^2} &= C_{55} \frac{\partial^2 \pi_z}{\partial x^2} + C_{44} \frac{\partial^2 \pi_z}{\partial y^2} + C_{33} \frac{\partial^2 \pi_z}{\partial z^2} + (C_{13} + C_{55}) \frac{\partial^2 \pi_x}{\partial z^2} + (C_{23} + C_{44}) \frac{\partial^2 \pi_x}{\partial z^2}. 
\end{align*}
\]

Note that, unlike the original elastic wave equation, pseudo-pure-mode wave equation does not contain mixed partial derivatives. This is a good news because it takes more computational cost to compute the mixed partial derivatives using a finite-difference algorithm with required accuracy. In the forthcoming text, we focus on demonstration of pseudo-pure-mode qP-wave equations for TI media while briefly supplement similar derivation for orthorhombic media in Appendix B.

**Pseudo-pure-mode qP-wave equation in VTI media**

For a VTI medium, there are only five independent parameters: \( C_{11}, C_{33}, C_{44}, C_{66} \) and \( C_{13} \), with \( C_{12} = C_{11} - 2C_{66}, C_{22} = C_{11}, C_{23} = C_{13} \) and \( C_{55} = C_{44} \). So we rewrite
equation 18 as,
\[
\rho \frac{\partial^2 \pi_x}{\partial t^2} = C_{11} \frac{\partial^2 \pi_x}{\partial x^2} + C_{66} \frac{\partial^2 \pi_x}{\partial y^2} + C_{44} \frac{\partial^2 \pi_x}{\partial z^2} + (C_{11} - C_{66}) \frac{\partial^2 \pi_y}{\partial x^2} + (C_{13} + C_{44}) \frac{\partial^2 \pi_z}{\partial x^2},
\]
\[
\rho \frac{\partial^2 \pi_y}{\partial t^2} = C_{66} \frac{\partial^2 \pi_y}{\partial x^2} + C_{11} \frac{\partial^2 \pi_y}{\partial y^2} + C_{44} \frac{\partial^2 \pi_y}{\partial z^2} + (C_{11} - C_{66}) \frac{\partial^2 \pi_x}{\partial y^2} + (C_{13} + C_{44}) \frac{\partial^2 \pi_z}{\partial y^2},
\]
\[
\rho \frac{\partial^2 \pi_z}{\partial t^2} = C_{44} \frac{\partial^2 \pi_z}{\partial x^2} + C_{44} \frac{\partial^2 \pi_z}{\partial y^2} + C_{33} \frac{\partial^2 \pi_z}{\partial z^2} + (C_{13} + C_{44}) \frac{\partial^2 \pi_x}{\partial z^2} + (C_{13} + C_{44}) \frac{\partial^2 \pi_y}{\partial z^2}.
\]
(19)

Since a TI material has cylindrical symmetry in its elastic properties, it is safe to sum the first two equations in equation (19) to yield a simplified form for wavefield modeling and RTM, namely
\[
\rho \frac{\partial^2 \pi_{xy}}{\partial t^2} = C_{11} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \pi_{xy} + C_{44} \frac{\partial^2 \pi_{xy}}{\partial z^2} + (C_{13} + C_{44}) \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \pi_z,
\]
\[
\rho \frac{\partial^2 \pi_z}{\partial t^2} = C_{44} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \pi_z + C_{33} \frac{\partial^2 \pi_z}{\partial z^2} + (C_{13} + C_{44}) \frac{\partial^2 \pi_{xy}}{\partial z^2},
\]
(20)

where \( \pi_{xy} = \pi_x + \pi_y \) represents the sum of the two horizontal components. Pure SH-waves horizontally polarize in the isotropic planes of VTI media with the polarization given by \((-k_y, k_x, 0)\), which implies \( ik_y \pi_x + ik_x \pi_y = 0 \), i.e., \( \pi_{xy} = 0 \), for the SH-wave. Therefore, the above partial summation (after the first-step projection) completes divergence operation and removes the SH-waves from the three-component pseudo-pure-mode qP-wave fields. As a result, there are no terms related to \( C_{66} \) any more in equation 20. Compared with original elastic wave equation, equation 20 further reduces the computational costs for 3D wavefield modeling and RTM for VTI media.

Applying the Thomsen notation [Thomsen, 1986],
\[
C_{11} = (1 + 2\epsilon)p v_{p0}^2,
\]
\[
C_{33} = p v_{s0}^2,
\]
\[
C_{44} = p v_{s0}^2,
\]
\[
(C_{13} + C_{44}) = p^2 (v_{p0}^2 - v_{s0}^2)(v_{p0}^2 - v_{s0}^2),
\]
(21)

the pseudo-pure-mode qP-wave equation can be expressed as,
\[
\frac{\partial^2 \pi_{xy}}{\partial t^2} = v_{px}^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \pi_{xy} + v_{s0}^2 \frac{\partial^2 \pi_{xy}}{\partial z^2} + \sqrt{(v_{p0}^2 - v_{s0}^2)}(v_{p0}^2 - v_{s0}^2) \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \pi_z,
\]
\[
\frac{\partial^2 \pi_z}{\partial t^2} = v_{s0}^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \pi_z + v_{p0}^2 \frac{\partial^2 \pi_z}{\partial z^2} + \sqrt{(v_{p0}^2 - v_{s0}^2)}(v_{p0}^2 - v_{s0}^2) \frac{\partial^2 \pi_{xy}}{\partial z^2},
\]
(22)

where \( v_{p0} \) and \( v_{s0} \) represent the vertical velocities of qP- and qSV-waves, \( v_{pn} = v_{p0} \sqrt{1 + 2\delta} \) represents the interval NMO velocity, \( v_{px} = v_{p0} \sqrt{1 + 2\epsilon} \) represents the horizontal velocity of qP-waves, \( \delta \) and \( \epsilon \) are the other two Thomsen coefficients. Unlike other coupled second-order systems derived from the dispersion relation of VTI
media (Zhou et al., 2006b), the wavefield components in equations 20 and 22 have clear physical meaning and their summation automatically produces scalar wavefields dominant of qP-wave energy. Equation 22 is also similar to a minimal coupled system (equation 30 in their paper) demonstrated by Fowler et al. (2010), except that it is now derived from a significant similarity transformation that helps to enhance qP-waves and suppress qS-waves (after summing the transformed wavefield components). This is undoubtedly useful for migration of conventional seismic data representing mainly qP-wave data.

We can also obtain a pseudo-acoustic coupled system by setting $v_{s0} = 0$ in equation 22, namely:

$$\frac{\partial^2 \bar{u}_{xy}}{\partial t^2} = (1 + 2\epsilon)v_{p0}^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\bar{u}_{xy} + \sqrt{1 + 2\delta}v_{p0}^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\bar{u}_z,$$

$$\frac{\partial^2 \bar{u}_z}{\partial t^2} = \frac{\partial^2 \bar{u}_z}{\partial z^2} + \sqrt{1 + 2\delta}v_{p0}^2\frac{\partial^2 \bar{u}_{xy}}{\partial z^2}. \tag{23}$$

The pseudo-acoustic approximation does not significantly affect the kinematic signatures but may distort the reflection, transmission and conversion coefficients (thus the amplitudes) of waves in elastic media.

If we further apply the isotropic assumption (setting $\delta = 0$ and $\epsilon = 0$) and sum the two equations in equation 23, we get the familiar constant-density acoustic wave equation:

$$\frac{\partial^2 \bar{u}}{\partial t^2} = v_p^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\bar{u}, \tag{24}$$

where $\bar{u} = \bar{u}_{xy} + \bar{u}_z$ represents the acoustic pressure wavefield, and $v_p$ is the propagation velocity of isotropic P-wave.

**Pseudo-pure-mode qP-wave equation in TTI media**

In the case of transversely isotropic media with a tilted symmetry axis, the elastic tensor loses its simple form. Written in Voigt notation, it contains nonzero entries in all four quadrants if expressed in global Cartesian coordinates $\mathbf{x} = (x, y, z)$. The generalization of pseudo-pure-mode wave equation to a tilted symmetry axis involves no additional physics but greatly complicates the algebra. One strategy to derive the wave equations in TTI media is to locally rotate the coordinate system so that its third axis coincides with the symmetry axis, and make use of the simple form in VTI media.

We introduce a transformation to a rotated coordinate system $\hat{\mathbf{x}} = (\hat{x}, \hat{y}, \hat{z})$,

$$\hat{\mathbf{x}} = \mathbf{R}^T \mathbf{x}, \tag{25}$$

where the rotation matrix $\mathbf{R}$ is dependent on the tilt angle $\theta$ and the azimuth $\varphi$ of
the symmetry axis, namely,

\[
\mathbf{R} = \begin{pmatrix}
  r_{11} & r_{12} & r_{13} \\
  r_{21} & r_{22} & r_{23} \\
  r_{31} & r_{32} & r_{33}
\end{pmatrix} = \begin{pmatrix}
  \cos \varphi & -\sin \varphi & 0 \\
  \sin \varphi & \cos \varphi & 0 \\
  0 & 0 & 1
\end{pmatrix} \begin{pmatrix}
  \cos \theta & 0 & -\sin \theta \\
  0 & 1 & 0 \\
  \sin \theta & 0 & \cos \theta
\end{pmatrix}.
\] (26)

So,

\[
r_{11} = \cos \theta \cos \varphi, \\
r_{12} = -\sin \varphi, \\
r_{13} = -\sin \theta \cos \varphi, \\
r_{21} = \cos \theta \sin \varphi, \\
r_{22} = \cos \varphi, \\
r_{23} = -\sin \theta \sin \varphi, \\
r_{31} = \sin \theta, \\
r_{32} = 0, \\
r_{33} = \cos \theta.
\] (27)

Assuming that the rotation operator \( \mathbf{R} \) varies slowly so that its spatial derivatives can be ignored, the second-order differential operators in the rotated coordinate system aligned with the symmetry axis are given as:

\[
\begin{align*}
\frac{\partial^2}{\partial x^2} &= r_{11}^2 \frac{\partial^2}{\partial x^2} + 2r_{11}r_{21} \frac{\partial^2}{\partial x \partial y} + 2r_{11}r_{31} \frac{\partial^2}{\partial x \partial z} + 2r_{21}r_{31} \frac{\partial^2}{\partial y \partial z}, \\
\frac{\partial^2}{\partial y^2} &= r_{12}^2 \frac{\partial^2}{\partial x^2} + 2r_{12}r_{22} \frac{\partial^2}{\partial y^2} + 2r_{12}r_{32} \frac{\partial^2}{\partial y \partial z} + 2r_{22}r_{32} \frac{\partial^2}{\partial y \partial z}, \\
\frac{\partial^2}{\partial z^2} &= r_{13}^2 \frac{\partial^2}{\partial x^2} + 2r_{13}r_{23} \frac{\partial^2}{\partial y \partial z} + 2r_{13}r_{33} \frac{\partial^2}{\partial y \partial z} + 2r_{23}r_{33} \frac{\partial^2}{\partial y \partial z}.
\end{align*}
\] (28)

Substituting these differential operators into the pseudo-pure-mode qP-wave equation of VTI media yields the pseudo-pure-mode qP-wave equation for TTI media in the global Cartesian coordinates. Likewise, the pseudo-pure-mode qP-wave equation in TTI media can be further simplified by applying the pseudo-acoustic approximation.

We must mention that, the above coordinate rotation in deriving the wave equations for TTI and tilted orthorhombic media (see Appendix B) should be improved to enhance numerical stability according to some significant insights provided in recent literatures (Duveneck and Bakker, 2011; Macesanu, 2011; Zhang et al., 2011; Bube et al., 2012).

**CORRECTION OF PROJECTION DEVIATION TO REMOVE QS-WAVES**

According to the theory of wave mode separation in anisotropic media, one needs to project the elastic wavefields onto the polarization direction to get the separated...
wavefields of the given mode (Dellinger and Etgen, 1990). Mathematically, this can be implemented through a dot product of the original vector wavefields and the polarization vector in the wavenumber domain (Dellinger and Etgen, 1990) or applying pseudo-derivative operators to the vector wavefields in the space-domain (Yan and Sava, 2009). However, the pseudo-pure-mode qP-wave equations are derived by a similarity transformation aiming to project the displacement wavefield onto the isotropic reference of qP-wave’s polarization vector. A partial mode separation has been automatically achieved during wavefield extrapolation using the pseudo-pure-mode qP-wave equations. For typical anisotropic earth media, thanks to the small departure of qP-wave’s polarization direction from its isotropic reference, the resulting pseudo-pure-mode wavefields are dominated by qP-wave energy and contaminated by residual qS-waves. To achieve a complete mode separation, we should further correct the projection deviations resulting from the differences between polarization and its isotropic reference. In other words, we split the conventional one-step wave mode separation for anisotropic media (Dellinger and Etgen, 1990; Yan and Sava, 2009) into two steps, of which the first one is implicitly achieved during extrapolating the pseudo-pure-mode wavefields and the second one is implemented after that using the approach that we will present immediately.

Taking VTI as an example, the deviation angle $\zeta$ between the polarization and propagation directions has a complicated nonlinear relation with anisotropic parameters and the phase angle (see Appendix C). According to its expression for weak anisotropic VTI media (Rommel, 1994; Tsvankin, 2001), it seems that the deviation is mainly affected by the difference between $\epsilon$ and $\delta$, the magnitude of $\delta$ (when $\epsilon - \delta$ stays the same) and the ratio of vertical velocities of qP- and qS-wave, as well as the phase angle. It is possible to design a filtering algorithm to suppress the residual qS-waves using the deviation angle given under the assumption of weak anisotropy. To completely remove the residual qS-waves and correctly separate the qP-waves for arbitrary anisotropy, we propose an accurate correction approach according to the deviation between polarization and wave vectors.

Considering equations 8, 9, 13, and 15, we first decompose the polarization vector of qP-wave $\mathbf{a}_p$ as follows:

$$\mathbf{a}_p = \mathbf{E}_p \mathbf{k},$$

where the deviation operator satisfies,

$$\mathbf{E}_p = \begin{pmatrix}
a_{px} / k_x & 0 & 0 \\
0 & a_{py} / k_y & 0 \\
0 & 0 & a_{pz} / k_z
\end{pmatrix}.$$  

This matrix can be constructed once the qP-wave polarization directions are determined based on the local medium properties at a grid point. For TI media, there are analytical expressions for the qP-wave polarization vectors (Dellinger, 1991). For other anisotropic media with lower symmetry (such as orthorhombic media), we have to numerically compute the polarization vectors using the Christoffel equation.
Then we correct the pseudo-pure-mode qP-wave fields $\tilde{u} = (\tilde{u}_x, \tilde{u}_y, \tilde{u}_z)^T$ using a wavenumber-domain filtering based on the deviation operator:

$$\tilde{u}_p = E_p \cdot \tilde{u},$$

and finally extract the scalar qP-wave data using

$$u_p = u_{px} + u_{py} + u_{pz}$$

after 3D inverse Fourier transforms. Here, the magnitude of the deviation operator for a certain wavenumber $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$ is a constant because this operator is computed by using the normalized wave and polarization vectors in equation 30. This ensures that for a certain wavenumber, the separated qP-waves are uniformly scaled. More important, this correction step thoroughly removes the residual qS-wave energy.

In heterogeneous anisotropic media, the polarization directions and thus the deviation operators vary spatially, depending on the local material parameters. To account for spatial variability, we propose an equivalent expression to equations 31 and 32 as a nonstationary filtering in the space domain at each location,

$$u_p = E_{px}(\bar{u}_x) + E_{py}(\bar{u}_y) + E_{pz}(\bar{u}_z)$$

where the pseudo-derivative operators $E_{px}(\cdot), E_{py}(\cdot),$ and $E_{pz}(\cdot)$ represent the inverse Fourier transforms of the diagonal elements in the deviation matrix $E_p$.

Figure 1 displays the wavenumber-domain operators of projection onto isotropic (reference) and anisotropic polarization vectors (namely $k$ and $a_p$) as well as the corresponding deviation operator $E_p$ for a 2D homogeneous VTI medium with $v_{p0} = 3000m/s$, $v_{s0} = 1500m/s$, $\epsilon = 0.25$ and $\delta = -0.25$. Note that $E_p$ is not simply the difference between $k$ and $a_p$, and $E_p$ becomes the identity operator in case of an isotropic medium. In the space-domain, projecting onto isotropic polarization directions is equivalent to a divergence operation using partial derivative operators, while projection onto polarization directions of qP-waves use operators that have the character of pseudo-derivative operators, due to anisotropy (see Figure 2). Figure 3 shows that the variation of the anisotropy changes the deviation operators greatly. The weaker the anisotropy, the more compact the deviation operators appear. The observation is basically consistent with the equation of polarization deviation angle for VTI media with weak anisotropy. The exact pseudo-derivative operators are very long series in the discretized space domain. Generally, the far ends of these operators have ignorable values even for strong anisotropy. Therefore, in practice, we could truncate the operators to make the spatial filters short and computationally efficient.

This procedure to separate qP-waves, although accurate, is computationally expensive, especially in 3D heterogeneous media. Like the computational problem in conventional wave mode separation from the anisotropic elastic wavefields (Yan and Sava, 2009, 2012), the spatial filtering to separate qP-waves is significantly more expensive than extrapolating the pseudo-pure-mode wavefields. In practice, we find that it is not necessary to apply the filtering at every time step. A larger time interval is...
allowed to save costs enormously, especially for RTM of multi-shot seismic data. According to our experiments, there is little difference between the two migrated images when the filtering is applied at every one and two time step (if only the filtered wavefields are used in the imaging procedure), although about three-fourths of the original computational cost are saved for the filtering in the latter case. Moreover, filtering at every three time step still produces an acceptable migrated image. We may further improve the efficiency of the filtering procedure by using the algorithm that resembles the phase-shift plus interpolation (PSPI) scheme recently used in anisotropic wave mode separation ([Yan and Sava, 2011]). Alternatively, we may greatly reduce the computational cost but guarantee the accuracy using the mixed (space-wavenumber) domain filtering algorithm based on low-rank approximation ([Cheng and Fomel, 2013]).

![Figure 1: Normalized wavenumber-domain operators of projection onto isotropic (reference) and anisotropic polarization vectors of qP-waves, and wavenumber-domain deviation operators in a 2D homogeneous VTI medium: $k$ (left), $a_p$ (middle) and $E_p$ (right); Top: x-component, Bottom: z-component.](qPwave/homovti.eta0.5/ adxNT,apxNT,apvxNT,adzNT,apzNT,apvzNT)

In kinematics, it seems that we can extract scalar qSV-wave fields from the pseudopure-mode qP-wave fields $\bar{u}$ by filtering according to the projection deviation defined by qSV-wave’s polarization and wave vector. However, unlike separation of the qP-wave mode, the large projection deviations for qSV-wave modes would result in significant discontinuities in the wavenumber-domain correction operators and strong tails extending off to infinity in the space domain. Accordingly, this reduces compactness of the spatial filters, which prohibits applying the same truncation as for qP-wave spatial filters to reduce computational cost. Computational tricks such as smoothing may result in distorted and incomplete separation. That is why we are developing a similar approach to simulate propagation of separated qS-wave modes based on their own pseudo-pure-mode wave equations and the corresponding projection deviation.
Figure 2: Space-domain operators of projecting onto isotropic (left) and anisotropic (middle) polarization vectors, and the corresponding deviation operators (right): Top: x-component, Bottom: z-component. Note that the operators are tapered before transforming into space-domain and the same gain is applied to all pictures to highlight the differences among these operators.

Figure 3: Comparison of the spatial domain deviation operators in VTI media with varied anisotropy strength: In all cases, $v_{p0} = 3000 \text{m/s}$, $v_{s0} = 1500 \text{m/s}$, and $\epsilon$ is fixed as 0.2. From left to right, $\delta$ is set as 0.2, 0.1, 0, -0.1, and -0.2, respectively. Top: x-components; Bottom: z-components. To highlight the differences, the same gain is applied to all pictures.
EXAMPLES

1. Simulating propagation of separated wave modes

1.1 Homogeneous VTI model

For comparison, we first apply the original anisotropic elastic wave equation to synthesize wavefields in a homogeneous VTI medium with weak anisotropy, in which $v_{p0} = 3000 \text{ m/s}$, $v_{s0} = 1500 \text{ m/s}$, $\epsilon = 0.1$, and $\delta = 0.05$. Figure 4a and 4b display the horizontal and vertical components of the displacement wavefields at 0.3 s. Then we try to simulate propagation of separated wave modes using the pseudo-pure-mode $qP$-wave equation (equation 22 in its 2D form). Figure 4c and 4d display the two components of the pseudo-pure-mode $qP$-wave fields, and Figure 4e displays their summation, i.e., the pseudo-pure-mode scalar $qP$-wave fields with weak residual $qSV$-wave energy. Compared with the theoretical wavefront curves (see Figure 4f) calculated on the base of group velocities and angles, pseudo-pure-mode scalar $qP$-wave fields have correct kinematics for both $qP$- and $qSV$-waves. We finally remove residual $qSV$-waves and get completely separated scalar $qP$-wave fields by applying the filtering to correct the projection deviation (Figure 4g).

Figure 4: Synthesized wavefields in a VTI medium with weak anisotropy: (a) $x$- and (b) $z$-components synthesized by original elastic wave equation; (c) $x$- and (d) $z$-components synthesized by pseudo-pure-mode $qP$-wave equation; (e) pseudo-pure-mode scalar $qP$-wave fields; (f) kinematics of $qP$- and $qSV$-waves; and (g) separated scalar $qP$-wave fields.
Then we consider wavefield modeling in a homogeneous VTI medium with strong anisotropy, in which $v_{p0} = 3000m/s$, $v_{s0} = 1500m/s$, $\epsilon = 0.25$, and $\delta = -0.25$. Figure 5 displays the wavefield snapshots at 0.3 s synthesized by using original elastic wave equation and pseudo-pure-mode qP-wave equation respectively. Note that the pseudo-pure-mode qP-wave fields still accurately represent the qP- and qSV-waves’ kinematics. Although the residual qSV-wave energy becomes stronger when the strength of anisotropy increases, the filtering step still removes these residual qSV-waves effectively.

Figure 5: Synthesized wavefields in a VTI medium with strong anisotropy: (a) x- and (b) z-components synthesized by original elastic wave equation; (c) x- and (d) z-components synthesized by pseudo-pure-mode qP-wave equation; (e) pseudo-pure-mode scalar qP-wave fields; (f) kinematics of qP- and qSV-waves; and (g) separated scalar qP-wave fields.

1.2 Two-layer TI model

This example demonstrates the approach on a two-layer TI model, in which the first layer is a very strong VTI medium with $v_{p0} = 2500m/s$, $v_{s0} = 1200m/s$, $\epsilon = 0.25$, and $\delta = -0.25$, and the second layer is a TTI medium with $v_{p0} = 3600m/s$, $v_{s0} = 1800m/s$, $\epsilon = 0.2$, $\delta = 0.1$, and $\theta = 30^\circ$. The horizontal interface between the two layers is positioned at a depth of 1.167 km. Figure 6a and 6d display the horizontal and vertical components of the displacement wavefields at 0.3 s. Using the pseudo-pure-mode qP-wave equation, we simulate equivalent wavefields on the same model. Figure 6b and 6e display the two components of the pseudo-pure-mode qP-wave fields at the same time step. Figure 6c and 6f display pseudo-pure-mode scalar qP-wave fields and separated qP-wave fields respectively. Obviously, residual qSV-waves (including transmitted, reflected and converted qSV-waves) are effectively removed,
and all transmitted, reflected as well as converted qP-waves are accurately separated after the projection deviation correction.

Figure 6: Synthesized wavefields on a two-layer TI model with strong anisotropy in the first layer and a tilted symmetry axis in the second layer: (a) x- and (d) z-components synthesized by original elastic wave equation; (b) x- and (e) z-components synthesized by pseudo-pure-mode qP-wave equation; (c) pseudo-pure-mode scalar qP-wave fields; (f) separated scalar qP-wave fields.

1.3 BP 2007 TTI model

Next we test the approach of simulating propagation of the separated qP-wave mode in a complex TTI model. Figure 7 shows parameters for part of the BP 2D TTI model. The space grid size is 12.5 m and the time step is 1 ms for high-order finite-difference operators. Here the vertical velocities for the qSV-wave are set as half of the qP-wave velocities. Figure 8 displays snapshots of wavefield components at the time of 1.4s synthesized by using original elastic wave equation and pseudo-pure-mode qP-wave equation. The two pictures at the bottom represent the scalar pseudo-pure-mode qP-wave and the separated qP-wave fields, respectively. The correction appears to remove residual qSV-waves and accurately separate qP-wave data including the converted qS-qP waves from the pseudo-pure-mode wavefields in this complex model.
Figure 7: Partial region of the 2D BP TTI model: (a) vertical qP-wave velocity, Thomsen coefficients (b) $\epsilon$ and (c) $\delta$, and (d) the tilt angle $\theta$.

1.4 Homogeneous 3D ORT model

Figure 9 shows an example of simulating propagation of separated qP-wave fields in a 3D homogeneous vertical ORT model, in which $v_{p0} = 3000\, m/s$, $v_{s0} = 1500\, m/s$, $\delta_1 = -0.1$, $\delta_2 = -0.0422$, $\delta_3 = 0.125$, $\epsilon_1 = 0.2$, $\epsilon_2 = 0.067$, $\gamma_1 = 0.1$, and $\gamma_2 = 0.047$. The first three pictures display wavefield snapshots at 0.5s synthesized by using pseudo-pure-mode qP-wave equation, according to equation B-3. As shown in Figure 9d, qP-waves again appear to dominate the wavefields in energy when we sum the three wavefield components of the pseudo-pure-mode qP-wave fields. As for TI media, we obtain completely separated qP-wave fields from the pseudo-pure-mode wavefields once the correction of projection deviation is finished (Figure 9e). By the way, in all above examples, we find that the filtering to remove qSV-waves does not require the numerical dispersion of the qS-waves to be limited. So there is no additional requirement of the grid size for qS-wave propagation. The effects of grid dispersion for the separation of low velocity qS-waves will be further investigated in the second article of this series.

2. Reverse-time migration of Hess VTI model

Our final example shows application of the pseudo-pure-mode qP-wave equation (i.e., equation 22 in its 2D form) to RTM of conventional seismic data representing mainly qP-wave energy using the synthetic data of SEG/Hess VTI model (Figure 10). In
Figure 8: Synthesized elastic wavefields on BP 2007 TTI model using original elastic wave equation and pseudo-pure-mode qP-wave equation respectively: (a) x- and (b) z-components synthesized by original elastic wave equation; (c) x- and (d) z-components synthesized by pseudo-pure-mode qP-wave equation; (e) pseudo-pure-mode scalar qP-wave fields; (f) separated scalar qP-wave fields.
Figure 9: Synthesized wavefield snapshots in a 3D homogeneous vertical ORT medium: (a) x-, (b) y- and (c) z-component of the pseudo-pure-mode qP-wave fields, (d) pseudo-pure-mode scalar qP-wave fields, (e) separated scalar qP-wave fields.
the original data set, there is no vertical velocity model for qSV-wave, namely $v_{s0}$. For simplicity, we first get this parameter by setting $\frac{v_{s0}}{v_{p0}} = 0.5$ anywhere. Figures 11a and 11b display the two components of the synthesized pseudo-pure-mode qP-wave fields, in which the source is located at the center of the windowed region of the original models. We observe that the summed wavefields (i.e., pseudo-pure-mode scalar qP-wave fields) contain quite weak residual qSV-wave energy (Figure 11c). For seismic imaging of qP-wave data, we try the finite nonzero $v_{s0}$ scheme (Fletcher et al., 2009) to suppress qSV-wave artifacts and enhance computation stability. Thanks to superposition of multi-shot migrated data, we obtain a good RTM result (Figure 12) using the common-shot gathers provided at http://software.seg.org, although spatial filtering has not been used to remove the residual qSV-wave energy. This example shows that the proposed pseudo-pure-mode qP-wave equation could be directly used for reverse-time migration of conventional single-component seismic data.

Figure 10: Part of SEG/Hess VTI model with parameters of (a) vertical qP-wave velocity, Thomsen coefficients (b) $\epsilon$ and (c) $\delta$.

Figure 11: Synthesized wavefields using the pseudo-pure-mode qP-wave equation in SEG/Hess VTI model: The three snapshots are synthesized by fixing the ratio of $v_{s0}$ to $v_{p0}$ as 0.5. The pseudo-pure-mode qP-wave fields (c) are the sum of the (a) x- and (b) z-components of the pseudo-pure-mode wavefields.
DISCUSSION

For the general anisotropic media, qP- and qS-wave modes are intrinsically coupled. The elastic wave equation must be solved at once to get correct kinematics and amplitudes for all modes. The scalar wavefields, however, are widely used with the help of wave mode separation or by using approximate equations derived from the elastic wave equation for many applications such as seismic imaging. As demonstrated in the theoretical parts, the pseudo-pure-mode wave equation is derived from the elastic wave equation through a similarity transformation to the Christoffel equation in the wavenumber domain. The components of the transformed wavefield essentially represent the spatial derivatives of the displacement wavefield components. This transformation preserves the kinematics of wave propagation but inevitably changes the phases and amplitudes for qP- and qS-waves as the elastic wave mode separation procedure using divergence-like and curl-like operations (Dellinger and Etgen, 1990; Yan and Sava, 2009; Zhang and McMechan, 2010). The filtering step to correct the projection deviation is indispensable for complete removing the residual qS-waves from the extrapolated pseudo-pure-mode qP-wave fields. This procedure does not change the phases and amplitudes of the scalar qP-waves because the deviation operator is computed using the normalized wave and polarization vectors.

In fact, it is not even clear what the correct amplitudes should be for "scalar anisotropy". Like the anisotropic pseudo-analytic methods (Etgen and Brandsberg-Dahl, 2009; Fomel et al., 2013; Zhan et al., 2012; Song and Alkhalifah, 2013), the pseudo-pure-mode wave equation may distort the reflection, transmission and conversion coefficients of the elastic wavefields when there are high-frequency perturbations.
in the velocity model. Therefore, the converted qP-waves remaining in the separated qP-wave fields only have reliable kinematics. What happens to the qP-wave’s amplitudes and how to make use of the converted qP-waves (for seismic imaging) on the base of the pseudo-pure-mode qP-wave equation need further investigation in our future research.

CONCLUSIONS

We have proposed an alternative approach to simulate propagation of separated wave modes in general anisotropic media. The key idea is splitting the one-step wave mode separation into two cascaded steps based on the following observations: First, the Christoffel equation derived from the original elastic wave equation accurately represents the kinematics of all wave modes; Second, various coupled second-order wave equations can be derived from the Christoffel equation through similarity transformations. Third, wave mode separation can be achieved by projecting the original elastic wavefields onto the given mode’s polarization directions, which are usually calculated based on the local material parameters using the Christoffel equation. Accordingly, we have derived the pseudo-pure-mode qP-wave equation by applying a similarity transformation aiming to project the elastic wavefield onto the wave vector, which is the isotropic references of qP-wave polarization for an anisotropic medium. The derived pseudo-pure-mode equations not only describe propagation of all wave modes but also implicitly achieve partial mode separation once the wavefield components are summed. As shown in the examples, the scalar pseudo-pure-mode qP-wave fields are dominated by qP-waves while the residual qS-waves are weaker in energy, because the projection deviations of qP-waves are generally far less than those of the qSV-waves. Synthetic example of Hess VTI model demonstrates successful application of the pseudo-pure-mode qP-wave equation to RTM for conventional seismic exploration. To completely remove the residual qS-waves, a filtering step has been proposed to correct the projection deviations resulting from the difference between polarization direction and its isotropic reference. In homogeneous media, it can be efficiently implemented by applying wavenumber domain filtering to each wavefield component. In heterogeneous media, nonstationary spatial filtering using pseudo-derivative operators are applied to finish the second step for wave mode separation. In a word, pseudo-pure-mode wave equations plus corrections of projection deviations provide us an efficient and flexible tool to simulate propagation of separated wave modes in anisotropic media.

In spite of the amplitude properties, this approach has some advantages over the classical solution combining elastic wavefield extrapolation and wave mode separation: First, the pseudo-pure-mode wave equations could be directly used for migration of seismic data recorded with single-component geophones without computationally expensive wave mode separation (as shown in the last example). Second, because partial wave mode separation is automatically achieved during wavefield extrapolation and the correction step to remove the residual qS-waves is optional depending on the
strength of anisotropy, our approach provides better flexibility for seismic modeling, migration and parameter inversion in practice; Third, computational cost is reduced at least one third for the 2D cases if the finite difference algorithms are used thanks to the simpler structure of pseudo-pure-mode wave equations (i.e., having no mixed derivative terms for VTI and vertically orthorhombic media). For the 3D TI media, computational cost is further reduced about one third because two instead of three equations are used to simulate wave propagation.

Unlike the pseudo-acoustic wave equations, pseudo-pure-mode wave equations have no approximation in kinematics and allow for $\epsilon < \delta$ provided that the stiffness tensor is positive-definite. Moreover, they provide a possibility to extract artifact-free separated wave mode during wavefield extrapolation. Although we focus on propagation of separated qP-waves using the pseudo-pure-mode qP-wave equation, our approach also works for qS-waves in TI media. This will be demonstrated in the second paper of this series.

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**APPENDIX A**

**PSEUDO-PURE-MODE QP-WAVE EQUATION FOR VERTICAL TI AND ORTHORHOMBIC MEDIA**

For vertical TI and orthorhombic media, the stiffness tensors have the same null components and can be represented in a two-index notation [Musgrave 1970] often called the Voigt notation as

$$
C = \begin{pmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{pmatrix}.
$$

(A-1)
For vertical orthorhombic tensor, the nine coefficients are independent, but the VTI tensor has only five independent coefficients with \( C_{12} = C_{11} - 2C_{66}, \ C_{22} = C_{11}, \ C_{23} = C_{13} \) and \( C_{55} = C_{44} \). The stability condition requires these parameters to satisfy the corresponding constraints (Helbig, 1994; Tsvankin, 2001). According to equations 3 and 4, the full elastic wave equation without the source terms is expressed as:

\[
\begin{align*}
\rho \frac{\partial^2 u_x}{\partial t^2} &= C_{11} \frac{\partial^2 u_x}{\partial x^2} + C_{66} \frac{\partial^2 u_x}{\partial y^2} + C_{55} \frac{\partial^2 u_x}{\partial z^2} + (C_{12} + C_{66}) \frac{\partial^2 u_y}{\partial x \partial y} + (C_{13} + C_{55}) \frac{\partial^2 u_z}{\partial x \partial z}, \\
\rho \frac{\partial^2 u_y}{\partial t^2} &= C_{66} \frac{\partial^2 u_y}{\partial x^2} + C_{22} \frac{\partial^2 u_y}{\partial y^2} + C_{44} \frac{\partial^2 u_y}{\partial z^2} + (C_{12} + C_{66}) \frac{\partial^2 u_x}{\partial x \partial y} + (C_{23} + C_{44}) \frac{\partial^2 u_z}{\partial y \partial z}, \\
\rho \frac{\partial^2 u_z}{\partial t^2} &= C_{55} \frac{\partial^2 u_z}{\partial x^2} + C_{44} \frac{\partial^2 u_z}{\partial y^2} + C_{33} \frac{\partial^2 u_z}{\partial z^2} + (C_{13} + C_{55}) \frac{\partial^2 u_x}{\partial x \partial z} + (C_{23} + C_{44}) \frac{\partial^2 u_y}{\partial y \partial z}.
\end{align*}
\]

Thus the corresponding Christoffel matrix in wavenumber domain satisfies

\[
\tilde{\Gamma} = \begin{pmatrix}
(C_{11}k_x^2 + C_{66}k_y^2 + C_{55}k_z^2) & (C_{12} + C_{66})k_xk_y & (C_{13} + C_{55})k_xk_z \\
(C_{12} + C_{66})k_xk_y & (C_{11}k_x^2 + C_{22}k_y^2 + C_{44}k_z^2) & (C_{23} + C_{44})k_yk_z \\
(C_{13} + C_{55})k_xk_z & (C_{23} + C_{44})k_yk_z & (C_{55}k_x^2 + C_{44}k_y^2 + C_{33}k_z^2)
\end{pmatrix}.
\]

According to equation 10, the Christoffel matrix after the similarity transformation is given as,

\[
\tilde{\Gamma} = \begin{pmatrix}
(C_{11}k_x^2 + C_{66}k_y^2 + C_{55}k_z^2) & (C_{12} + C_{66})k_xk_y^2 & (C_{13} + C_{55})k_xk_z^2 \\
(C_{12} + C_{66})k_x^2k_y & (C_{11}k_x^2 + C_{22}k_y^2 + C_{44}k_z^2) & (C_{23} + C_{44})k_yk_z^2 \\
(C_{13} + C_{55})k_x^2k_z & (C_{23} + C_{44})k_y^2k_z & (C_{55}k_x^2 + C_{44}k_y^2 + C_{33}k_z^2)
\end{pmatrix}.
\]

Finally, we obtain the pseudo-pure-mode qP-wave equation (i.e., equation 18) by inserting equation A-4 into equation 12 and applying an inverse Fourier transform.

**APPENDIX B**

**PSEUDO-PURE-MODE QP-WAVE EQUATION IN ORTHORHOMBIC MEDIA**

One of the most common reasons for orthorhombic anisotropy in sedimentary basins is a combination of parallel vertical fractures and vertically transverse isotropy in the background medium (Wild and Crampin, 1991; Schoenberg and Helbig, 1997). Vertically orthorhombic models have three mutually orthogonal planes of mirror symmetry that coincide with the coordinate planes \([x_1, x_2], [x_1, x_3]\) and \([x_2, x_3]\). Here we assume \(x_1\) axis is the x-axis (and used as the symmetry axis), \(x_2\) the y-axis, and \(x_3\) the z-axis.
Using the Thomsen-style notation for orthorhombic media (Tsvankin, 1997):

\[ v_{p0} = \sqrt{\frac{C_{33}}{\rho}}, \]
\[ v_{s0} = \sqrt{\frac{C_{55}}{\rho}}, \]
\[ \epsilon_1 = \frac{C_{22} - C_{33}}{2C_{33}}, \]
\[ \delta_1 = \frac{(C_{33} + C_{44})^2 - (C_{33} - C_{44})^2}{2C_{33}(C_{33} - C_{44})}, \]
\[ \gamma_1 = \frac{C_{66} - C_{55}}{2C_{55}}, \]
\[ \epsilon_2 = \frac{C_{11} - C_{33}}{2C_{33}}, \]
\[ \delta_2 = \frac{(C_{13} + C_{55})^2 - (C_{33} - C_{55})^2}{2C_{33}(C_{33} - C_{55})}, \]
\[ \gamma_2 = \frac{C_{66} - C_{44}}{2C_{44}}, \]
\[ \delta_3 = \frac{(C_{12} + C_{66})^2 - (C_{11} - C_{66})^2}{2C_{11}(C_{11} - C_{66})}, \]

and

\[ v_{px1} = v_{p0} \sqrt{1 + 2\epsilon_1}, \]
\[ v_{px2} = v_{p0} \sqrt{1 + 2\epsilon_2}, \]
\[ v_{sx1} = v_{s0} \sqrt{1 + 2\gamma_1}, \]
\[ v_{sx2} = v_{s0} \sqrt{1 + 2\gamma_2}, \]
\[ v_{pn1} = v_{p0} \sqrt{1 + 2\delta_1}, \]
\[ v_{pn2} = v_{p0} \sqrt{1 + 2\delta_2}, \]
\[ v_{pn3} = v_{p0} \sqrt{1 + 2\delta_3}, \]
the pseudo-pure-mode qP-wave equation (equation 18) is rewritten as,

\[
\frac{\partial^2 \tilde{\pi}_x}{\partial t^2} = v^2_{px2} \frac{\partial^2 \tilde{\pi}_x}{\partial x^2} + v^2_{s11} \frac{\partial^2 \tilde{\pi}_x}{\partial y^2} + v^2_{p0} \frac{\partial^2 \tilde{\pi}_x}{\partial z^2} + \sqrt{(v^2_{px2} - v^2_{s11})(1 + 2\epsilon_2)} \frac{\partial^2 \tilde{\pi}_y}{\partial x^2} \\
+ \sqrt{(v^2_{p0} - v^2_{s12})(v^2_{pm2} - v^2_{s12})} \frac{\partial^2 \tilde{\pi}_z}{\partial y^2},
\]

\[
\frac{\partial^2 \tilde{\pi}_y}{\partial t^2} = v^2_{s11} \frac{\partial^2 \tilde{\pi}_y}{\partial x^2} + v^2_{px1} \frac{\partial^2 \tilde{\pi}_y}{\partial y^2} + v^2_{s12} \frac{\partial^2 \tilde{\pi}_y}{\partial z^2} + \sqrt{(v^2_{px1} - v^2_{s11})(1 + 2\epsilon_2)} \frac{\partial^2 \tilde{\pi}_x}{\partial y^2} \\
+ \sqrt{(v^2_{p0} - v^2_{s12})(v^2_{pm2} - v^2_{s12})} \frac{\partial^2 \tilde{\pi}_z}{\partial z^2},
\]

\[
\frac{\partial^2 \tilde{\pi}_z}{\partial t^2} = v^2_{s12} \frac{\partial^2 \tilde{\pi}_z}{\partial x^2} + v^2_{px2} \frac{\partial^2 \tilde{\pi}_z}{\partial y^2} + v^2_{p0} \frac{\partial^2 \tilde{\pi}_z}{\partial z^2} + \sqrt{(v^2_{px2} - v^2_{s12})(1 + 2\epsilon_2)} \frac{\partial^2 \tilde{\pi}_x}{\partial y^2} \\
+ \sqrt{(v^2_{p0} - v^2_{s12})(v^2_{pm2} - v^2_{s12})} \frac{\partial^2 \tilde{\pi}_y}{\partial z^2},
\]

(B-3)

where \(v_{p0}\) represents the vertical velocity of qP-wave, \(v_{s0}\) represents the vertical velocity of qS-waves polarized in the \(x_1\) direction, \(\epsilon_1\), \(\delta_1\) and \(\gamma_1\) represent the VTI parameters \(\epsilon\), \(\delta\) and \(\gamma\) in the \([y, z]\) plane, \(\epsilon_2\), \(\delta_2\) and \(\gamma_2\) represent the VTI parameters \(\epsilon\), \(\delta\) and \(\gamma\) in the \([x, z]\) plane, \(\delta_3\) represents the VTI parameter \(\delta\) in the \([x, y]\) plane. \(v_{px1}\) and \(v_{px2}\) are the horizontal velocities of qP-wave in the symmetry planes normal to the \(x\) and \(y\)-axis, respectively. \(v_{pm1}\), \(v_{pm2}\) and \(v_{pm3}\) are the interval NMO velocities in the three symmetry planes, and \(v_{s12} = v_{s0}\sqrt{|1 + 2\epsilon_1|/(1 + 2\gamma_2)}\).

Setting \(v_{s0} = 0\), we further obtain the pseudo-acoustic coupled system in a vertically orthorhombic media,

\[
\frac{\partial^2 \tilde{\pi}_x}{\partial t^2} = v^2_{px2} \frac{\partial^2 \tilde{\pi}_x}{\partial x^2} + (1 + 2\epsilon_2) \sqrt{1 + 2\delta_3} v^2_{p0} \frac{\partial^2 \tilde{\pi}_y}{\partial x^2} + \sqrt{1 + 2\delta_2} v^2_{p0} \frac{\partial^2 \tilde{\pi}_z}{\partial x^2},
\]

\[
\frac{\partial^2 \tilde{\pi}_y}{\partial t^2} = (1 + 2\epsilon_2) \sqrt{1 + 2\delta_3} v^2_{p0} \frac{\partial^2 \tilde{\pi}_x}{\partial y^2} + (1 + 2\epsilon_1) v^2_{p0} \frac{\partial^2 \tilde{\pi}_y}{\partial y^2} + \sqrt{1 + 2\delta_1} v^2_{p0} \frac{\partial^2 \tilde{\pi}_z}{\partial y^2},
\]

\[
\frac{\partial^2 \tilde{\pi}_z}{\partial t^2} = \sqrt{1 + 2\delta_2} v^2_{p0} \frac{\partial^2 \tilde{\pi}_x}{\partial z^2} + \sqrt{1 + 2\delta_1} v^2_{p0} \frac{\partial^2 \tilde{\pi}_y}{\partial z^2} + v^2_{p0} \frac{\partial^2 \tilde{\pi}_z}{\partial z^2}.
\]

Note that this equation does not contain any of the parameters \(\gamma_1\) and \(\gamma_2\) that describe the shear-wave velocities in the directions of the \(x\) and \(y\)-axis, respectively. Evidently, kinematic signatures of qP-waves in pseudo-acoustic orthorhombic media depend on just five anisotropic coefficients \((\epsilon_1, \epsilon_2, \delta_1, \delta_2\) and \(\delta_3)\) and the vertical velocity \(v_{p0}\).

In the presence of dipping fracture, we need to extend the vertically orthorhombic symmetry to a more complex form, i.e. orthorhombic media with tilted symmetry planes. Similar to TTI media, we locally rotate the coordinate system to make use of the simple form of the pseudo-pure-mode wave equations in vertically orthorhombic media. Since the physical properties are not symmetric in the local \([x_1, x_2]\) plane, we need three angles to describe the rotation (Zhang and Zhang, 2011). Two angles, \(\theta\) and \(\varphi\), are used to define the vertical axis at each spatial point as we did for the
symmetry axis in TTI model. The third angle \( \alpha \) is introduced to rotate the stiffness tensor on the local plane and to represent the orientation of the fracture system in a VTI background or the orientation of the first fracture system of two orthogonal ones in an isotropic background.

The second-order differential operators in the rotated coordinate system are expressed in the same forms as in equation (28), but the rotation matrix is now given by,

\[
R = \begin{pmatrix}
\cos \varphi & -\sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\cos \theta & 0 & \sin \theta \\
0 & 1 & 0 \\
-\sin \theta & 0 & \cos \theta
\end{pmatrix}
\begin{pmatrix}
\cos \alpha & -\sin \alpha & 0 \\
\sin \alpha & \cos \alpha & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

(B-5)

where

\[
\begin{align*}
r_{11} &= \cos \theta \cos \varphi \cos \alpha - \sin \varphi \sin \alpha, \\
r_{12} &= -\cos \theta \cos \varphi \sin \alpha - \sin \varphi \cos \alpha, \\
r_{13} &= \sin \theta \cos \varphi, \\
r_{21} &= \cos \theta \sin \varphi \cos \alpha + \cos \varphi \sin \alpha, \\
r_{22} &= -\cos \theta \sin \varphi \sin \alpha + \cos \varphi \cos \alpha, \\
r_{23} &= \sin \theta \sin \varphi, \\
r_{31} &= -\sin \theta \cos \alpha, \\
r_{32} &= \sin \theta \sin \alpha, \\
r_{33} &= \cos \theta.
\end{align*}
\]

(B-6)

Substituting the second-order differential operators into the rotated coordinate system for those in the pseudo-pure-mode qP-wave equation of vertically orthorhombic media yields the pseudo-pure-mode qP-wave equation of tilted orthorhombic media in the global Cartesian coordinates.

**APPENDIX C**

**DEVIAITION BETWEEN PHASE NORMAL AND POLARIZATION DIRECTION OF QP-WAVES IN VTI MEDIA**

For VTI media, [Dellinger (1991)] presents an expression of the deviation angle \( \zeta \) between the phase normal (with phase angle \( \psi \)) and the polarization direction of qP-waves, namely

\[
\sin^2(\zeta) = \frac{1}{2} + \frac{(2s - 1)t_1 - t_2}{2(t_2 \chi - t_1^2)} \sqrt{t_1^2 - t_2 \chi},
\]

(C-1)
where
\[
\begin{align*}
  s &= \sin^2(\psi), \\
  t_1 &= s(C_{33} + C_{11} - 2C_{44}) - C_{33} + C_{44} \\
  &= s\rho[v_{p0}^2 + (1 + 2\epsilon)v_{p0}^2 - 2v_{s0}^2] - \rho v_{p0}^2 + \rho v_{s0}^2, \\
  t_2 &= 4s(s - 1)\chi, \\
  \chi &= C_{13} + C_{44} \\
  &= \rho \sqrt{(v_{p0}^2 - v_{s0}^2)(v_{pm}^2 - v_{s0}^2)}.
\end{align*}
\]

Equation C-1 indicates that the deviation angle has a complicated nonlinear relation with anisotropic parameters and the phase angle. The relationship is rather lengthy and does not easily reveal the features caused by anisotropy. Hence we use an alternative expression under a weak anisotropy assumption (Rommel, 1994; Tsvankin, 2001),

\[
\zeta = \left[\delta + 2(\epsilon - \delta)\sin^2 \psi\right] \sin 2\psi \\
2(1 - \frac{v_{s0}^2}{v_{p0}^2})
\]

(C-3)

It appears that the deviation angle is mainly affected by the difference between \(\epsilon\) and \(\delta\), the magnitude of \(\delta\) (when \(\epsilon - \delta\) stays the same) and the ratio of vertical velocities of qP- and qS-wave, as well as the phase angle.
REFERENCES

media: Geophysics, 69, 576–582.


