1	Stochastic inversion of seismic PP and PS data for reservoir parameter			
2	estimation			
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4	Shortened Title: Stochastic inversion of PP and PS data			
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ABSTRACT

2 We investigate the value of isotropic seismic converted-wave (i.e., PS) data for reservoir 3 parameter estimation using stochastic approaches based on the floating-grain rock-4 physics model. We first perform statistical analysis on a simple two-layer model built on 5 actual borehole logs and compare the relative value of PS data versus AVO gradient data 6 for estimating floating-grain fraction. We find that PS data are significantly more 7 informative than AVO gradient data for estimating floating-grain fraction in terms of 8 likelihood functions, and the combination of PS and AVO gradient data together with full 9 PP stack data provides the maximal value for the reservoir parameter estimation. To 10 evaluate the value of PS data under complex situations, we develop a hierarchical 11 Bayesian model to combine seismic PP and PS data and their associated time registration. 12 We extend a model-based Bayesian method developed previously for inverting seismic 13 PP data by including PS responses and time registration as additional data and two-way 14 PS travel time and PS reflectivity as additional variables. We apply the method to a 15 synthetic six-layer model that closely mimics real field scenarios. The case study results 16 show that PS data provide more information than AVO gradient data for estimating 17 floating-grain fraction, porosity, net-to-gross, and layer thicknesses when their 18 corresponding priors are weak.

INTRODUCTION

2 Multicomponent seismic surveying has been used for hydrocarbon exploration for 3 decades because it can capture the seismic wave-field more completely than conventional single-element techniques (Stewart et al., 2002). Although several types of energy 4 5 conversion may occur when seismic waves pass through the underlying earth, transmitted 6 or multiple conversions generally have much lower amplitudes than the P-down and S-up 7 reflection (Rodriguez-Saurez, 2000). Consequently, among many applications of multi-8 component seismic data, the use of converted-wave or PS images receives much more 9 attention (Stewart et al., 2002; Mahmoudian and Margrave, 2004; Veire and Landro, 10 2006). However, the high acquisition cost of collecting multicomponent seismic data 11 compared to conventional seismic surveys and the challenge in processing 12 multicomponent data, makes the use of converted-wave data as a routine practice 13 difficult.

14 The interest in using multicomponent seismic data again for hydrocarbon 15 applications is inspired by recent advances in seismic data acquisition technologies, such 16 as ocean-bottom seismometer techniques (e.g., ocean-based cables and ocean-based nodes) (Hardage et al., 2011; Pacal, 2012). With the use of new techniques, 17 18 multicomponent seismic data can be collected more reliably compared to conventional 19 seismic survey techniques. Another major reason for using multicomponent seismic data 20 is the need to estimate spatially-distributed ductile fraction (Glinsky et al., 2013), and to 21 characterize fractures for unconventional resources because shear-wave splitting provides 22 an effective approach to image fracture orientation and density (Bale et al., 2013). There 23 are many other successful applications of converted-wave data, such as time-lapse monitoring of geomechanical changes (Davis et al., 2013), and reservoir characterization
 (Brettwood et al., 2013).

3 In this study, we use stochastic approaches to investigate the value of converted-4 wave data for reservoir parameter estimation based on a floating-grain rockphysics model 5 developed by DeMartini and Glinsky (2006). The model is well-documented (Gunning 6 and Glinsky, 2007) and appropriate for porous sedimentary rocks in which some solid 7 materials are "floating" or not involved in loading support because it can explain the 8 observed variation in P-wave velocity versus density trends, and lack of variation in the 9 P-wave velocity versus S-wave velocity trends. The rockphysics relationship can be 10 modified and applied to unconventional shale resource exploration as done by Glinsky et 11 al. (2013), where the media is considered as a binary mixing of brittle and ductile 12 materials and ductile fraction plays the same role as floating-grain fraction.

13 We employ stochastic methods in the study because they have many advantages 14 over traditional deterministic approaches in reservoir parameter estimation using multiple 15 geophysical data sets when dealing with complex issues involving uncertainty (Chen et 16 al., 2008). We start from analyzing a simple two-layer model by comparing the relative 17 value of full PS versus AVO gradient data for estimating floating-grain fraction 18 according to their likelihoods when both rockphysics models and seismic data are subject 19 to uncertainty. We then focus on more complicated cases involving multiple layers and 20 develop a hierarchical Bayesian model to combine seismic PP and PS data and their 21 associated time registration.

We extend the model-based Bayesian method developed by Gunning and Glinsky (2004) for inverting seismic AVO data, by revising their open-source Java codes (i.e.,

'Delivery') to allow isotropic converted-wave responses and PS event time registration as additional data. We use the same rock physics models and Markov chain Monte Carlo (MCMC) (Gilks et al., 1996) sampling strategies as Delivery. Since this study is built on the previous work, the subsequent descriptions will be focused on the new development and applications, and the details of other parts can be found in Gunning and Glinsky (2004).

7

ROCKPHYSICS MODEL AND ANALYSIS OF TWO-LAYER MODELS

8 Floating-grain rockphysics model

9 We use the floating-grain rockphysics models developed by Demartini and Glinsky 10 (2006) and Gunning and Glinsky (2007) to link reservoir parameters to seismic attributes. 11 In the model, the subsurface is considered as a binary mixture of reservoir members (say 12 sand) and non-reservoir members (say shale). For sand, we assume that some solid 13 materials are "floating" in pore space and seismic properties (i.e., seismic P- and S-wave 14 velocity and density) can be characterized by two fundamental parameters. One of them 15 is loading depth (z), which is measure of effective pressure; the other is floating-grain 16 fraction (x). The general model is given below

17
$$v_p = a_{vp} + b_{vp}z + c_{vp}x + \varepsilon_{vp}, \qquad (1)$$

18
$$v_s = a_{vs} + b_{vs}v_p + \varepsilon_{vs}, \qquad (2)$$

19
$$\rho = a_{\rho} + b_{\rho} v_{\rho} + c_{\rho} x + \varepsilon_{\rho}. \tag{3}$$

In equations 1-3, symbols v_{ρ} , v_{s} , and ρ represent seismic P- and S-wave velocity and density, and symbols $\varepsilon_{v\rho}$, ε_{vs} , and ε_{ρ} represent uncertainty associated with their 1 corresponding regression equations. We assume that ε_{vp} , ε_{vs} , and ε_{ρ} have Gaussian 2 distributions with zero mean and variance of σ_{vp}^2 , σ_{vs}^2 , and σ_{ρ}^2 , respectively.

We rewrite equations 2-3 in terms of loading depth z and floating-grain fraction x
as follows

$$v_{s} = (a_{vs} + a_{vp}b_{vs}) + b_{vs}b_{vp}z + b_{vs}c_{vp}x + (b_{vs}\varepsilon_{vp} + \varepsilon_{vs}),$$
(4)

$$\rho = (a_{\rho} + a_{\nu p}b_{\rho}) + b_{\rho}b_{\nu p}z + (b_{\rho}c_{\nu p} + c_{\rho})x + (b_{\rho}\varepsilon_{\nu p} + \varepsilon_{\rho}).$$
(5)

We can see that in the rockphysics model, seismic properties linearly depend on the
reservoir parameters with uncertainty.

We can use different relationships for shale because seismic properties in shale do not depend on floating-fraction. As it has been done in Gunning and Glinsky (2007), we drop floating-grain fraction from equations 1 and 4 and use the power-law form of the Gardner relationship (Gardner et al., 1974) for density, i.e., $\rho = av_p^b + \varepsilon_\rho$, where both *a* and *b* are coefficients. By fitting actual borehole logs from suitable field sites, we obtain all those coefficients and their associated standard errors for sand and shale members. Table 1 is a summary of all those values.

16 **Reflectivity coefficients**

We use the linearized Zoeppritz approximations (Aki and Richard, 1980) for small
contrasts and angles to obtain PP and PS reflectivity coefficients at an interface, which
are given below:

20
$$R_{pp}(\theta) = \frac{1}{2} \left(\frac{\Delta v_p}{v_p} + \frac{\Delta \rho}{\rho} \right) + \frac{1}{2} \left[\frac{\Delta v_p}{v_p} - 4r_{sp}^2 \left(\frac{\Delta \rho}{\rho} + 2\frac{\Delta v_s}{v_s} \right) \right] \theta^2, \quad (6)$$

$$R_{ps}(\theta) = -\frac{1}{2} \left[\frac{\Delta \rho}{\rho} + 2r_{sp} \left(\frac{\Delta \rho}{\rho} + 2\frac{\Delta v_s}{v_s} \right) \right] \theta.$$
(7)

In equations 6 and 7, v_p = (v_{p1} + v_{p2})/2, v_s = (v_{s1} + v_{s2})/2, ρ = (ρ₁ + ρ₂)/2, r_{sp} = v_s/v_p,
Δv_p = v_{p2} - v_{p1}, Δv_s = v_{s2} - v_{s1}, and Δρ = ρ₂ - ρ₁, where (v_{p1}, v_{s1}, ρ₁) and (v_{p2}, v_{s2}, ρ₂)
are P- and S-wave velocity and density in the layers above and below the interface.
Symbol θ is the PP incident angle in the unit of radius. The PP and PS reflectivities have
the fourth and third order of accuracy in terms of the incident angle.
For ease of description, we let A₀ be the first term in equation 6, A₁ be the first

8 term in equation 7 excluding θ, and A₂ be the second term in equation 6 excluding θ².
9 We thus have the following relationship:

10
$$\begin{pmatrix} A_{0} \\ A_{1} \\ A_{2} \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 & 0 \\ -1/2 - r_{sp} & 0 & -2r_{sp} \\ -2r_{sp}^{2} & 1/2 & -4r_{sp}^{2} \end{pmatrix} \begin{pmatrix} \Delta \rho / \rho \\ \Delta v_{p} / v_{p} \\ \Delta v_{s} / v_{s} \end{pmatrix}.$$
(8)

We use the capital letter **A** to represent the vector on the left side of equation 8 and use \mathbf{M}_a and $\Delta \mathbf{C}$ represent the matrix and the vector on the right side of the equation. Thus equation 8 becomes $\mathbf{A} = \mathbf{M}_a \Delta \mathbf{C}$. These notations will be used in the subsequent text.

14 Synthetic two-layer model

1

To demonstrate the value of PS data, we start from a simple two-layer model based on actual borehole logs from Gunning and Glinsky (2007), with the first layer being shale and the second layer being sand whose rockphysics models are given in Table 1. Since we focus on estimation of floating-grain fraction in the sand layer, we fix the loading depth as $z_1 = 17,060$ ft and $z_2 = 17,457$ ft for the first and second layers. By using the 1 shale regression equations with coefficients given in Table 1, we have $v_{p1} = 10,756$ ft/s,

2 $v_{s1} = 5,245$ ft/s, and $\rho_1 = 2.49$ g/cc. By using equations 1, 4, and 5, we can get

3
$$\Delta \rho = (a_{\rho} + a_{\nu p} b_{\rho} + b_{\nu p} b_{\rho} z_2 - \rho_1) + (b_{\rho} c_{\nu p} + c_{\rho}) x + (\varepsilon_{\rho} + b_{\rho} \varepsilon_{\nu p}), \qquad (9)$$

$$\Delta v_p = (a_{vp} + b_{vp} z_2 - v_{p1}) + c_{vp} x + \varepsilon_{vp}, \qquad (10)$$

5
$$\Delta v_{s} = (a_{vs} + a_{vp}b_{vs} + b_{vp}b_{vs}z_{2} - v_{s1}) + b_{vs}c_{vp}x + (\varepsilon_{vs} + b_{vs}\varepsilon_{vp}).$$
(11)

6 Let

4

7
$$\begin{cases} w_{\rho} = a_{\rho} + a_{vp}b_{\rho} + b_{vp}b_{\rho}z_{2} - \rho_{1} \\ w_{vp} = a_{vp} + b_{vp}z_{2} - v_{p1} \\ w_{vs} = a_{vs} + a_{vp}b_{vs} + b_{vp}b_{vs}z_{2} - v_{s1} \end{cases}$$
(12)

8 We have

9
$$\begin{pmatrix} \Delta \rho / \rho \\ \Delta v_{p} / v_{p} \\ \Delta v_{s} / v_{s} \end{pmatrix} = \begin{pmatrix} w_{\rho} / \rho \\ w_{vp} / v_{p} \\ w_{vs} / v_{s} \end{pmatrix} + \begin{pmatrix} (c_{\rho} + b_{\rho}c_{vp}) / \rho \\ c_{vp} / v_{p} \\ b_{vs}c_{vp} / v_{s} \end{pmatrix} x + \begin{pmatrix} (\varepsilon_{\rho} + b_{\rho}\varepsilon_{vp}) / \rho \\ \varepsilon_{vp} / v_{p} \\ (\varepsilon_{vs} + b_{vs}\varepsilon_{vp}) / v_{vs} \end{pmatrix}.$$
(13)

10 Let \mathbf{W}_0 , \mathbf{W}_1 , and $\boldsymbol{\varepsilon}_w$ represent the first, second, and third vectors on the right side of 11 equation 13. We get $\Delta \mathbf{C} = \mathbf{W}_0 + \mathbf{W}_1 x + \boldsymbol{\varepsilon}_w$. By assuming that the errors in equations 1-3 12 are independent, we can obtain the following covariance matrix $\boldsymbol{\Sigma}_w$

13
$$\Sigma_{w} = \begin{pmatrix} (\sigma_{\rho}^{2} + b_{\rho}^{2} \sigma_{vp}^{2}) / \rho^{2} & b_{\rho} \sigma_{vp}^{2} / (\rho v_{p}) & b_{\rho} b_{vs} \sigma_{vp}^{2} / (\rho v_{s}) \\ b_{\rho} \sigma_{vp}^{2} / (\rho v_{p}) & \sigma_{vp}^{2} / v_{p}^{2} & b_{vs} \sigma_{vp}^{2} / (v_{p} v_{s}) \\ b_{\rho} b_{vs} \sigma_{vp}^{2} / (\rho v_{s}) & b_{vs} \sigma_{vp}^{2} / (v_{p} v_{s}) & (\sigma_{vs}^{2} + b_{vs}^{2} \sigma_{vp}^{2}) / v_{vs}^{2} \end{pmatrix}.$$
(14)

14 Synthetic seismic data and likelihood function

For the purpose of this analysis, we consider the PP and PS reflectivities at the interface as data. Specifically, we use a full PP stack with an incident angle of zero and a full PS stack with an incident angle of θ , and an AVO gradient stack with an incident angle of θ. Let vector **R**_m be the data with additive Gaussian random noise ε_m. We thus
 have (see Appendix A for the detailed derivation)

3
$$\mathbf{R}_{m} = \mathbf{M}_{\theta} \mathbf{M}_{a} \Delta \mathbf{C} + \boldsymbol{\varepsilon}_{m} = \mathbf{M}_{\theta} \mathbf{M}_{a} (\mathbf{W}_{0} + \mathbf{W}_{1} x) + (\boldsymbol{\varepsilon}_{m} + \mathbf{M}_{\theta} \mathbf{M}_{a} \boldsymbol{\varepsilon}_{w}), \qquad (15)$$

4 where the angle dependent matrix \mathbf{M}_{θ} is defined as follows:

$$\mathbf{M}_{\theta} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \theta & 0 \\ 0 & 0 & \theta^2 \end{bmatrix}.$$
 (16)

6 The second term on the right side of equation 15 is residuals, which include two 7 parts, i.e., the measurement errors and the uncertainty caused by the rockphysics model. 8 Since we assume both parts have multivariate Gaussian distribution, their summation also 9 has a multivariate Gaussian distribution (Stone, 1995). Let Σ_m be the covariance matrix of measurement errors and Σ_w be the covariance matrix of uncertainty in rockphysics 10 models. The combined covariance thus is given by $\sum_{c} = \mathbf{M}_{\theta} (\sum_{m} + \mathbf{M}_{a} \sum_{w} \mathbf{M}_{\theta}^{T}) \mathbf{M}_{\theta}^{T}$, where 11 Σ_w is given by equation 14. Consequently, the likelihood function of x given data \mathbf{R}_m is 12 13 a multivariate Gaussian distribution as follows:

14
$$f(\mathbf{R}_{m} | x) \propto \left| \sum_{c} \right|^{-1/2} \times \exp\left\{ -(\mathbf{R}_{m} - \mathbf{M}_{\theta} \mathbf{M}_{a} \mathbf{W}_{0} - \mathbf{M}_{\theta} \mathbf{M}_{a} \mathbf{W}_{1} x)^{T} \sum_{c}^{-1} (\mathbf{R}_{m} - \mathbf{M}_{\theta} \mathbf{M}_{a} \mathbf{W}_{0} - \mathbf{M}_{\theta} \mathbf{M}_{a} \mathbf{W}_{1} x) \right\}.$$
(17)

15 Model comparison

5

We compare the estimation results by using four different combinations of seismic data by specifying their angle-dependent matrices: (1) using only the full PP stack, (2) using the full PP and PS stacks, (3) using the full PP and AVO gradient stacks, and (4) using all the seismic data (see Appendix B to find angle-dependent matrix for each case). 1 Their corresponding data can be represented by $\mathbf{R}_m^{(1)}$, $\mathbf{R}_m^{(2)}$, $\mathbf{R}_m^{(3)}$, and $\mathbf{R}_m^{(4)}$. To avoid the 2 effects of prior distribution on floating-grain fraction, we focus on the likelihood 3 functions $f(\mathbf{R}_m^{(k)} | x)$ (k = 1, 2, 3, 4) for those models.

4 Figure 1 compares the likelihood functions for the true floating-grain fraction being 5 0.0 (Figure 1a) and 0.035 (Figure 1b). The noise levels for all the data are equal to 0.01 in 6 the unit of reflection coefficients (RFC). The black, green, red, and blue curves represent the likelihoods obtained using (1) the full PP stack only, (2) the full PP and AVO 7 8 gradient stacks, (3) the full PP and PS stacks, and (4) all the seismic data. As we expect, 9 the true values have the maximum likelihood in both cases. It is clear that the likelihoods 10 of using the full PP and AVO gradient data (green curves) are considerably larger than 11 those of using the full PP stack only (black curves). The likelihoods of using the full PP 12 and full PS stacks (red curves) are significantly larger than those of using the full PP and 13 AVO gradient stacks (green curves). This suggests that the combination of the full PP 14 and PS stacks are more informative for estimating floating-grain fraction than that of full 15 PP and AVO gradient stacks. When we use all the data, we can get the largest likelihoods 16 (blue curves). This implies that the full PS and AVO gradient stacks may complement to 17 each other to some degree. In addition, we can see that the clean sand (Figure 1a) overall 18 has larger likelihoods with the maximum of 24 than the sand with floating grain (Figure 19 1b) with the maximum of 14.

The above comparison depends on the noise levels in the seismic data. In practice, full PS and AVO gradient stacks are typically have larger errors than full PP stacks. To investigate the effects of noise on the likelihood analysis, we vary noise levels in both full PS and AVO gradient stacks from 0.01 RFC to 0.1 RFC while fixing the noise level of the full PP stack as 0.01 RFC. We first calculate the maximum likelihoods for each
 combination of seismic data and then normalize the results by the values of using the full
 PP stack only to get the following likelihood ratios

4
$$r_{k} = \frac{\max\{f(\mathbf{R}_{m}^{(k)} \mid x)\}}{\max\{f(\mathbf{R}_{m}^{(1)} \mid x)\}}.$$
 (18)

5 Figure 2 shows the likelihood ratios for the true floating-grain fraction of 0.0 and 6 0.035. The green, red, and blue curves are the likelihood ratios of using the full PP and 7 AVO gradient stacks, the full PP and PS stacks, and all the seismic data. Generally, as the 8 noise levels in the full PS and AVO gradient data increase, the likelihood ratios decrease 9 and approach to 1, the result of using the full PP stack only. Additionally, we can see the 10 likelihood ratios of using the full PP and PS stacks always have larger likelihood ratios 11 than those of using full PP and gradient stacks and the likelihood ratios of using all the 12 data always have the largest values. This means that the combination of full PP and full 13 PS stacks is more informative than that of full PP and AVO gradient stacks even under 14 larger noise levels.

15

BAYESIAN MODEL FOR MULTIPLE LAYERS

16 Hierarchical Bayesian models

Although analysis of two-layer models allows us to understand the value of PS data for floating-grain fraction estimation, it is just marginal analysis of relative changes of compaction and floating-grain fraction across an interface under simple conditions. In the case of multiple layers, we need to develop a hierarchical Bayesian model to combine seismic PP and PS data and their time registration. This model is an extension of the model-based Bayesian method by Gunning and Glinsky (2004) with converted wave responses and PS time registration as additional data and two-way PS travel time and PS
 reflectivity as additional unknowns.

We consider effective seismic P-wave and S-wave velocity (\mathbf{v}_p and \mathbf{v}_s) and 3 density (ρ), and seismic PP and PS reflectivity (\mathbf{R}_{pp} and \mathbf{R}_{ps}) as unknowns. They are 4 5 functions of rock physics parameters through suitable rock physics models. We consider PP traveltime (\mathbf{t}_{pp}) as a primary unknown, and both layer thickness (\mathbf{d}) and PS 6 traveltime (\mathbf{t}_{ps}) can be derived from the PP traveltime and associated effective seismic 7 attributes. The data used for inversion include seismic PP and PS full-waveforms (\mathbf{S}_{pp} , 8 and \mathbf{S}_{ps}) and PP and PS event registration time (\mathbf{T}_{pp} and \mathbf{T}_{ps}). If available, we can also 9 10 include other types of information from nearby boreholes, such as depth constraints (\mathbf{D}_{b}) . 11 Figure 3 shows all the unknowns, available data, and their relationships; the dashed 12 rectangle highlights our extension to Delivery. Specifically, we add two unknowns related to converted wave (i.e., \mathbf{t}_{ps} , and \mathbf{R}_{ps}) and two types of new data sets (i.e., \mathbf{T}_{ps} 13 14 and S_{ps}). Following the direct graphical model, we have the following hierarchical

15 Bayesian model:

$$f(\boldsymbol{\alpha}, \mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{d}, \mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho}, \mathbf{R}_{pp}, \mathbf{R}_{ps} | \mathbf{S}_{pp}, \mathbf{S}_{ps}, \mathbf{T}_{pp}, \mathbf{T}_{ps}, \mathbf{D}_{b})$$

$$\propto f(\mathbf{S}_{pp} | \mathbf{t}_{pp}, \mathbf{R}_{pp}) f(\mathbf{S}_{ps} | \mathbf{t}_{ps}, \mathbf{R}_{ps}) f(\mathbf{T}_{pp} | \mathbf{t}_{pp})$$

$$16 \qquad \qquad \times f(\mathbf{T}_{ps} | \mathbf{t}_{ps}) f(\mathbf{D}_{b} | \mathbf{d}) f(\mathbf{R}_{pp} | \mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho}) \qquad (19)$$

$$\times f(\mathbf{R}_{ps} | \mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho}) f(\mathbf{d} | \mathbf{t}_{pp}, \mathbf{v}_{p}) f(\mathbf{t}_{ps} | \mathbf{t}_{pp}, \mathbf{v}_{s}, \mathbf{v}_{s})$$

$$\times f(\mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho} | \boldsymbol{\alpha}) f(\boldsymbol{\alpha}) f(\mathbf{t}_{pp}).$$

Equation 19 defines a joint posterior probability distribution function of all unknown parameters up to a normalizing constant. The first five terms on the right side of the equation are the likelihood functions of available data, which link data to the associated unknowns; other terms on the right side are the prior probability distributions,
 which are derived from other sources of information, such as rockphysics models. We
 define all the likelihood functions and prior distributions in a similar way to Delivery (see
 Gunning and Glinsky, 2004). In the following, we only describe the new development.

5 Equation 19 is a general Bayesian model for combining seismic PP and converted-6 wave data, and we can simplify or vary the equation in different ways depending on 7 specific applications. For example, we can consider PP and PS reflectivities as functions of \mathbf{v}_p , \mathbf{v}_s , and $\boldsymbol{\rho}$, but ignore their associated uncertainties and consider depth \mathbf{d} as a 8 9 function of P-wave velocity and two-layer PP travel time. Since in Bayesian statistics 10 (Bernardo and Smith, 2000), data affect unknowns only through likelihood functions, we can use statistics $Q(S_{pp}, S_{ps})$ of seismic data S_{pp} and S_{ps} in the Bayesian model, for 11 12 example, the rotation and truncation of original seismic data through principal component analysis (Venables and Ripley, 1999) or other methods. Consequently, we can have the 13 14 following Bayesian model:

15

5

$$f(\mathbf{\alpha}, \mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho} | \mathbf{S}_{pp}, \mathbf{S}_{ps}, \mathbf{T}_{pp}, \mathbf{T}_{ps})$$

$$\propto f(\mathbf{Q} | \mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho}) f(\mathbf{T}_{pp} | \mathbf{t}_{pp}) f(\mathbf{T}_{ps} | \mathbf{t}_{ps})$$

$$\times f(\mathbf{t}_{ps} | \mathbf{t}_{pp}, \mathbf{v}_{p}, \mathbf{v}_{s}) f(\mathbf{v}_{p}, \mathbf{v}_{s}, \boldsymbol{\rho} | \boldsymbol{\alpha}) f(\boldsymbol{\alpha}) f(\mathbf{t}_{pp}).$$
(20)

16 Likelihood function of seismic data

We describe a general form of the likelihood function in terms of statistics of seismic data, with the likelihood function of original seismic data as a special case of the form. Let $\mathbf{G}(\mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \mathbf{\rho})$ be the response vector of a suitable forward model that links seismic statistics \mathbf{Q} to unknowns. Let vector $\mathbf{\varepsilon}_{m}$ represent the residuals. We assume 1 that the residuals have the multivariate Gaussian distribution with zero mean and the 2 covariance matrix of Σ_m . We thus have

$$f(\mathbf{Q} | \mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \mathbf{\rho}) = (2\pi)^{-k/2} \left| \Sigma_{m} \right|^{1/2}$$

$$\times \exp\left(-\frac{1}{2} \left(\mathbf{Q} - \mathbf{G}(\mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \mathbf{\rho})^{T} \Sigma_{m}^{-1} \left(\mathbf{Q} - \mathbf{G}(\mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \mathbf{\rho})\right)\right).$$
(21)

In equation 21, k is the dimension of the multivariate Gaussian distribution and $|\Sigma_m|$ is the determinant of the covariance matrix Σ_m . One of the main advantages of using statistics in equation 21 is that we can have more options in defining likelihood functions so that we make their residuals uncorrelated.

8 Likelihood functions of PP and PS event time registration

9 The use of event time registration as data is one of main advantages of Delivery, as 10 well as the current extension, because PP event time is directly related to P-wave velocity 11 and PS event time directly related to P-wave and S-wave velocity. They provide 12 additional information to constrain the estimates of P-wave and S-wave velocity beyond 13 the reflectivity-based PP and PS full-waveforms.

Traditional methods for joint inversion of PP and PS data are primarily based on mapping of PS data to PP time (or domain conversion), in which PS data are considered as additional seismic stacks. Although this approach is simple to implement, it suffers from difficulties, such as wavelet distortion (Bansal and Matheney, 2010), because the conversion of PS time to PP time needs interval seismic P-to-S velocity ratios, which are not known *a priori*. In this study, we avoid the PP-to-PS domain conversion and use PS data directly in the PS time domain. We pick a PS event from PS seismograms that has a good correspondence with a PP event in the PP seismograms along the same profile, and we refer it to as the master PS horizon. In the PS forward simulation, we calculate all the PS times relative to the master horizon. The relative PP and PS time for a given layer is calculated by:

7
$$\Delta t_{ps} = \frac{1}{2} \left(1 + \frac{v_p}{v_s} \right) \Delta t_{pp} \,. \tag{22}$$

8 In equation 22, both PP and PS velocity are interval velocity and are unknown; they will
9 be estimated in inversion procedures.

10 The likelihood functions of PP and PS event registration time are determined by 11 assuming the errors have multivariate Gaussian distribution. Let Σ_{pp} and Σ_{ps} be the 12 covariance matrices of PP and PS event time, respectively. We have the following 13 likelihood functions after ignoring the constant:

14

$$f(\mathbf{T}_{pp} | \mathbf{t}_{pp}) \propto (2\pi)^{-k_{1}/2} \left| \Sigma_{pp} \right|^{-1/2} \exp\left(-\frac{1}{2} \left(\mathbf{T}_{pp} - \mathbf{t}_{pp}\right)^{T} \Sigma_{pp}^{-1} \left(\mathbf{T}_{pp} - \mathbf{t}_{pp}\right)\right), \text{ and}$$

$$f(\mathbf{T}_{ps} | \mathbf{t}_{ps}) \propto (2\pi)^{-k_{2}/2} \left| \Sigma_{ps} \right|^{-1/2} \exp\left(-\frac{1}{2} \left(\mathbf{T}_{ps} - \mathbf{t}_{ps}\right)^{T} \Sigma_{ps}^{-1} \left(\mathbf{T}_{ps} - \mathbf{t}_{ps}\right)\right).$$
(23)

15 In equation 23, k_1 and k_2 are the dimensions of \mathbf{T}_{pp} and \mathbf{T}_{ps} ; $|\Sigma_{pp}|$ and $|\Sigma_{ps}|$ are the 16 determinants of the covariance matrix Σ_{pp} and Σ_{ps} .

17 Conditionals of unknowns and Markov chain Monte Carlo sampling methods

We use Markov chain Monte Carlo methods to draw many samples from the jointdistribution given in equation 20. To do this, we need first derive conditional

distributions of each type of unknowns given all other variables and data. The
normalizing constants of each conditional are irrelevant when we use MCMC methods to
draw samples. Therefore, we only need to keep the term on the right of equation 20 to get
its conditional, which are given below:

5
$$f(\mathbf{t}_{pp} | \cdot) \propto f(\mathbf{Q} | \mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \mathbf{\rho}) f(\mathbf{T}_{pp} | \mathbf{t}_{pp}) f(\mathbf{t}_{ps} | \mathbf{t}_{pp}, \mathbf{v}_{p}, \mathbf{v}_{s}) f(\mathbf{t}_{pp}),$$
(24)

6
$$f(\mathbf{t}_{ps} | \cdot) \propto f(\mathbf{Q} | \mathbf{t}_{pp}, \mathbf{t}_{ps}, \mathbf{v}_{p}, \mathbf{v}_{s}, \mathbf{\rho}) f(\mathbf{T}_{ps} | \mathbf{t}_{ps}) f(\mathbf{t}_{ps} | \mathbf{t}_{pp}, \mathbf{v}_{p}, \mathbf{v}_{s}),$$
(25)

7
$$f(\mathbf{v}_{p},\mathbf{v}_{s},\boldsymbol{\rho}|\cdot) \propto f(\mathbf{Q}|\mathbf{t}_{pp},\mathbf{t}_{ps},\mathbf{v}_{p},\mathbf{v}_{s},\boldsymbol{\rho})f(\mathbf{t}_{ps}|\mathbf{t}_{pp},\mathbf{v}_{p},\mathbf{v}_{s})f(\mathbf{v}_{p},\mathbf{v}_{s},\boldsymbol{\rho}|\boldsymbol{\alpha}),$$
(26)

$$f(\boldsymbol{\alpha}|\cdot) \propto f(\mathbf{v}_p, \mathbf{v}_s, \boldsymbol{\rho}|\boldsymbol{\alpha}) f(\boldsymbol{\alpha}).$$
(27)

9 For equations 24-26, we cannot obtain analytical forms of those conditionals 10 because PP and PS registration time and seismic attributes \mathbf{v}_p , \mathbf{v}_s , and $\boldsymbol{\rho}$ are nonlinear 11 functions of other variables. We have to use MCMC methods (Gilks et al., 1996) to draw 12 many samples from the joint posterior distribution.

13 In equation 27, we use the floating-grain rockphysics model given in equations 1-3 14 to link layered seismic attributes to their corresponding reservoir parameters, which is a linear function in this case. Let vector **r** be the combined vector of \mathbf{v}_p , \mathbf{v}_s , and $\boldsymbol{\rho}$ 15 arranged by the layer indices and vector $\boldsymbol{\alpha}$ be the corresponding reservoir parameters. 16 We thus have $\mathbf{r} = \boldsymbol{\mu}_r + \mathbf{H}\boldsymbol{\alpha} + \boldsymbol{\varepsilon}_r$, where vector $\boldsymbol{\varepsilon}_r$ represents uncertainty associated with 17 18 the linear relationship. We assume that it has a multivariate Gaussian distribution with 19 zero mean and the covariance matrix of Σ_r . The detailed derivation and specific forms 20 are given in Appendix C.

1 If we use a multivariate Gaussian prior for $\boldsymbol{\alpha}$, i.e., $f(\boldsymbol{\alpha}) \sim N(\boldsymbol{\mu}_p, \boldsymbol{\Sigma}_p)$, we can 2 obtain the analytical formula of posterior distribution, $f(\boldsymbol{\alpha}|\cdot) \sim N(\boldsymbol{\mu}_u, \boldsymbol{\Sigma}_u)$, which is 3 given below

$$\begin{cases} \boldsymbol{\Sigma}_{u}^{-1} = \mathbf{H}^{T} \boldsymbol{\Sigma}_{r}^{-1} \mathbf{H} + \boldsymbol{\Sigma}_{p}^{-1}, \\ \boldsymbol{\Sigma}_{u}^{-1} \mathbf{u} = \mathbf{H}^{T} \boldsymbol{\Sigma}_{r}^{-1} (\mathbf{r} - \boldsymbol{\mu}_{r}) + \boldsymbol{\Sigma}_{p}^{-1} \boldsymbol{\mu}_{p}. \end{cases}$$
(28)

We can obtain many samples of the joint posterior distribution given in equation 20
by using MCMC sampling methods. In this study, we draw many samples using revised
Delivery developed by Gunning and Glinsky (2004).

8

CASE STUDY OF MULTIPLE LAYERS

9 We use the second example of Gunning and Glinsky (2007) to demonstrate the 10 benefits of including converted-wave data into estimation of floating-grain fraction. 11 Figure 4 shows various logs from an actual borehole, including P- and S-wave velocity, 12 density, P- and S-wave velocity ratios, and P-wave impedance. According to the logs, we 13 can build a synthetic model with six layers, which are (1) hard marl, (2) soft marl, (3) 14 shale, (4) upper sand, (5) shale, and (6) lower sand from shallow to deep (see Figure 5). 15 Both upper and lower sands are oil reservoirs with an oil saturation of 0.62 and 16 thicknesses of 700 ft and 360 ft, respectively. Table 2 summarizes the main reservoir 17 parameters and effective seismic properties. As shown in the table, layers 4 and 6 have 18 relatively low Vp/Vs ratios and include the floating-grain fraction of 0.035.

19 PP and PS reflectivities and synthetic seismic data

We use the PP and PS wavelets typical of those derived from field borehole logs
 for sparse-spike inversion using the method by Sassen and Glinsky (2013). The PP and
 PS wavelets have the peak frequencies of 23 Hz and 13 Hz, respectively (see Figure 6).

4 We generate synthetic PP and PS data by first using equations 6 and 7 to calculate 5 PP and PS reflectivities and then convolve the reflectivities with their corresponding 6 wavelets. Table 3 shows the calculated full PP and the angle-weighted full PS and AVO 7 gradient reflectivities at the five interfaces. As we can see that at the top interface, the 8 reflectivities of the full PP stack (incident angle = 0 degrees) is very strong, which 9 dominates the reflection from other deeper layers. Except at the interface between Layers 10 4 and 5, the magnitudes of PS reflectivities at all the interfaces are much larger than those 11 of their corresponding AVO gradient reflectivities. We convolve those reflectivities with 12 the given wavelets to get seismic full waveforms. Figure 7 shows the synthetic seismic 13 data without noise added, where full PP and AVO gradient stacks are in the PP time domain whereas the full PS stacks are in the PS time domain. For inversion, we assume 14 15 those data have uncorrelated Gaussian random noise with the standard deviation of 0.01 RFC. 16

17 **Priors for the inversion**

Since our main focus is on the demonstration of the value of PS data for reservoir parameter estimation, we mainly focus on the estimation of floating-grain fraction and net-to-gross in the upper and lower pay layers. Similar to Gunning and Glinsky (2007), we first consider prior $X \sim N(0.02, 0.03^2)$, which is a strong prior for the true floatinggrain fraction of 0.035. Secondly, we consider a weak prior $X \sim N(0.0, 0.05^2)$, which give significant prior probability to the zero floating-grain fraction or clean sand. For net1 to-gross (NG), we also consider two types of priors: (1) $NG \sim N(0.6, 0.1^2)$, and (2) 2 $NG \sim N(0.5, 0.3^2)$.

Since we use model-based inversion methods, we can set a wide range of priors and consider many parameters as unknowns. For example, we assume that PP travel time to each interface has the normal distribution with the true values as mean and 10 milliseconds as the standard deviation. We assume the uncertainty in the thickness of Layer 4 is 70 ft (i.e., 10% of the thickness) and 20 ft for other layers. We increase the uncertainty of Layer 4 later to study its sensitivity to PS data.

9 Inversion cases

To demonstrate the usefulness of PS data for improving parameter estimation, we invert synthetic seismic data under the following four scenarios: (1) using only the full PP stack, (2) using full PP and AVO gradient stacks, (3) using full PP and PS stacks, and (4) using all the seismic data. We compare the posterior estimates of each case with their corresponding prior distributions to evaluate the benefit of using PS data.

Since the above comparisons usually depend on inversion situation, we consider the following three factors: (1) prior on floating-grain fraction (i.e., $X \sim N(0.02, 0.03^2)$ or $X \sim N(0.0, 0.05^2)$), (2) prior on net-to-gross (i.e., $NG \sim N(0.6, 0.1^2)$ or $NG \sim N(0.5, 0.3^2)$). We consider two sets of noise levels. The first one is that all seismic data have a noise level of 0.01 RFC, and the other is that PP full stacks have a noise level of 0.01 RFC, but AVO gradient stacks and PS stacks have a noise level of 0.02 RFC. By changing priors and noise levels, we obtain many sets of posterior distributions. We use MCMC methods to draw 20,000 samples and keep the later half for analysis. With the use of those samples, we can obtain wide ranges of statistics, such as means, medians, modes, density functions, and predictive intervals. In the following several subsections, we selectively report our results.

6 Estimation of floating-grain fraction, porosity, and net-to-gross

7 We compare the estimates of reservoir parameters (i.e., floating-grain fraction, net-8 to-gross, and porosity) under different prior distributions. To investigate the effects of 9 priors about floating-grain fraction, we use a strong prior about net-to-gross, i.e., 10 $NG \sim N(0.6, 0.1^2)$, and noise levels for all the data types of 0.01 RFC. This implies we 11 have the same quality for all the seismic data. We will explore the effects of noise levels 12 later on.

13 Figure 8 compares the posterior probability densities (PDFs) of floating-grain 14 fraction, porosity, and net-to-gross with their corresponding prior PDFs (black curves) for 15 Layer 4 (i.e., upper-pay layer). The red, green, and blue curves represent the posterior 16 PDFs after conditioning on full PP stacks, full PP and AVO gradient stacks, and full PP 17 and PS stacks, respectively. For floating-grain fraction, even under the good prior (i.e, $X \sim N(0.02, 0.03^2)$), the mode of the prior probability corresponds to the zero floating-18 19 grain fraction or clean sand (see black curves in Figure 8a). After conditioning to seismic 20 data (i.e., full PP, full PP plus AVO stacks, or full PP plus full PS stacks), the modes of 21 the posterior PDFs corresponds to the true values 0.035 (see the red, green, and blue 22 curves), with the results of using full PP and PS stacks slightly better than other two. As shown in Figure 9a, if we use a biased prior to clean sand, say $X \sim N(0.0, 0.05^2)$, the 23

posterior estimates of floating-grain fraction using PP data only and using both full PP and AVO gradient stacks provide biased results (i.e., clean sand). However, the combination of full PP and full PS data provides correct estimates of the true value.

4 We can get similar results for comparison of porosity PDFs (see Figure 8b vs. 5 Figure 9b). Under the good prior of floating-grain fraction, the modes of the posterior 6 estimates for all the combinations of seismic data correspond to the true value quite well. 7 But under the biased prior of floating-grain fraction, only the posterior estimates obtained 8 using full PP and PS stacks provide good estimates of porosity. Since we use a very strong prior about net-to-gross (i.e., $NG \sim N(0.6, 0.1^2)$) for the true value of 0.65, we 9 10 expect the updating of the prior is minimal for all the posterior estimates (see Figure 8c 11 and Figure 9c).

We have similar comparisons of posterior PDFs for the lower-pay layer (i.e., Layer 6). Although overall the posterior estimates of floating-grain fraction and porosity are worse than those in the upper-pay layer, the combination of full PP and PS stack provides more information than full PP stacks only or the combination of full PP and AVO gradient stacks for updating the priors of floating-grain fraction and porosity.

17 Effects of the prior about net-to-gross and noise levels in seismic data

To explore the effects of prior about net-to-gross, we use less informative prior (i.e., $NG \sim N(0.5, 0.3^2)$) for net-to-gross and good prior about floating-grain fraction $(X \sim N(0.02, 0.03^2))$. Since the properties in the lower-pay layer are much less sensitive to seismic data, we only do the comparison for the upper-pay layer. Similar to what we found earlier, the combination of full PP and PS stacks significantly improve the estimates of floating-grain fraction and porosity (see the blue curves over the red and green curves in Figure 10a and 10b). Unlike previous comparison in Figures 8c and 9c,
 we found the combined use of full PP and PS stacks in this case significantly improve the
 estimates of net-to-gross when it has significant uncertainty (see Figure 10c).

4 In reality, it is more difficult to collect and process full PS and AVO gradient 5 stacks compared to full PP data. Therefore, they are likely subject to larger noise. To 6 explore the effects of noise levels on reservoir parameter estimation, we let the prior of floating-grain fraction be $X \sim N(0.02, 0.03^2)$ and let net-to-gross prior be 7 8 $NG \sim N(0.6, 0.1^2)$. We set the noise level in full PP stacks as 0.01 RFC but noise levels 9 in full PS and AVO gradient stacks as 0.02 RFC. Figure 11 shows the posterior PDFs of 10 floating-grain fraction, porosity and net-to-gross. Although the estimated results slightly 11 worse than those obtained using noise levels of 0.01 RFC (see Figure 8), the conclusions 12 remain the same.

13 Comparison of discrepancies between the estimated and the true values

Since we use sampling-based methods for inversion, we can obtain many samples of other variables as given in equation 20, such as effective P-wave and S-wave velocity, density, layer-thickness, etc. With the use of those samples, we can not only visually compare prior and posterior PDFs but also calculate a wide range of statistics. In the previous comparisons, we qualitatively compare the posterior estimates with their corresponding priors. To demonstrate the value of PS data, in this section, we quantitatively compare the estimated results with their true values.

We first compare the difference between the estimated median and the true value, which measures how accurate a chosen point estimator (in this case, median) to the true value of a given parameter. Figure 12a compares the differences between the estimated

1 floating-grain fraction, porosity, and net-to-gross values with their true values. The priors for floating-grain fraction is $X \sim N(0.0, 0.05^2)$ and for net-to-gross is $NG \sim N(0.6, 0.1^2)$, 2 3 and the noise levels are 0.01 RFC for full PP stacks and 0.02 for other data sets. We 4 normalize the results by the difference obtained from prior distributions. For net-to-gross, 5 as we demonstrated early, under the good prior, the estimated medians do not improve 6 the prior medians. The value slightly over 1.0 may reflect the effects of noise in seismic 7 data or sampling variations during the inversion procedure. For floating-grain fraction 8 and porosity, when conditioning to full PP data, the differences are significantly reduced 9 (see the triangles and circles corresponding to 'R0' in Figure 12a). When adding AVO 10 gradient stacks, the improvement is minimal (see the points corresponding to 'ROR2' in 11 Figure 12a), but adding PS data leads to significant reduction (see the points 12 corresponding to 'R0R1').

13 Figure 12b compares the differences for effective P-wave and S-wave velocity, 14 effective density, and layer thickness. For effective P-wave velocity and density, 15 conditioning to seismic full PP data significantly improves the accuracy, and further 16 adding AVO gradients or PS data does not lead significantly reduction. However, for 17 effective S-wave velocity and layer thickness, either adding AVO gradient stacks or PS 18 stacks lead to further reduction of the discrepancies, but adding of PS data causes more 19 reduction. For density (see the crosses in Figure 12b), adding full PS data does not lead to 20 significant reduction in uncertainty. This is because for the current case study, after 21 conditioning to full PP data, the uncertainty is already very small, leaving less room for 22 further improvement.

23 Comparison of widths of uncertainty bounds

1 The MCMC-based methods also allow us to quantitatively compare the uncertainty 2 associated with all the estimation. In this study, we calculate the widths of 95% predictive 3 intervals. Similar to the comparison of the discrepancies, we normalize the results by 4 those obtained from the prior PDFs.

5 Figure 13 shows the results for reservoir parameters and for effective parameters. 6 For reservoir parameters (i.e., floating-grain fraction, porosity, and net-to-gross), the 7 reduction of uncertainty is small and the maximum values are around 20%. The use of 8 various combinations of seismic data seems not make significant difference. For P-wave 9 velocity and density, after conditioning to full PP data, adding AVO gradient data or full 10 data does not lead further significant reduction. However, for S-wave velocity and layer 11 thickness, adding PS data causes significantly more reduction in the uncertainty than 12 adding AVO gradient data.

13 Comparison of predictive probabilities

In the previous sections, we compare the discrepancy between the estimated and true value and the widths of uncertainty bounds, both of which just compare one aspect of posterior PDFs. A better evaluation is to compare the predictive probabilities of a small interval around the true value, which is given by

18
$$\operatorname{Prob}(\theta \in [(1-\varepsilon)\theta^{True}, (1+\varepsilon)\theta^{True}] | \operatorname{Data}).$$
 (29)

In equation 29, we set $\varepsilon = 2.5\%$ for effective density and 5% for other parameters because the posterior density has much smaller uncertainty compared to other effective properties. The large predictive probability means that the data provide stronger evidence to support the occurrence of the true values. Again, we normalize the probabilities by the prior predictive probability.

1 Figure 14a compares the predictive probability ratios of floating-grain fraction, 2 porosity, and net-to-gross. These results are more consistent than those shown in Figures 3 12a and 13a as the ratios of net-to-gross are very close to 1.0. This means that for the tight prior of net-to-gross ($NG \sim N(0.5, 0.1^2)$), the updating is ignorable. For floating-4 5 grain fraction and porosity, the use of full PP stacks significantly increases the predictive 6 probabilities. Adding AVO gradient stacks does not cause significant improvement. 7 However, adding of full PS stacks leads to significant improvement again. Figure 14b 8 shows the similar comparison for effective P-wave and S-wave velocity, effective 9 density, and layer thickness. Similar statements to Figures 12b and 13b hold, but their 10 results are more consistent.

11

CONCLUSIONS

12 We started from likelihood analysis of a simple two-layer model based on the 13 floating-grain rock-physics model and found that seismic PS data are significantly more 14 informative than AVO gradient data for reservoir parameter estimation. This motivated 15 us to develop a hierarchical Bayesian model to combine PP and PS data under more 16 complicated cases (e.g., multiple layers, a large number of unknowns, etc). We inverted 17 PS data directly in the PS time domain unlike many previous methods that first convert 18 PS time to PP time and then invert PS data in the PP time domain. The alignment of PP 19 and PS time was carried out by identifying a common reflection interface and using the 20 PP and PS time to the interface as references. This avoids many difficulties caused by the 21 conversion of PS time to PP time, such as the distortion of wavelets, and the requirement 22 of knowing internal P-wave to S-wave velocity ratios a-priori. Since we considered PS time registration as data in the model, we can obtain more information during the joint
 inversion compared to previous methods for inverting PS data.

3

3 We revised the open-source Java codes, 'Delivery', to implement the developed 4 Bayesian model by adding converted wave responses and PS time registration as 5 additional data and two-way PS travel time and PS reflectivity as additional unknowns. 6 We took advantage of general structures for model setup, convenient ways to specify priors, efficient MCMC sampling methods, and various post analysis tools. We 7 8 demonstrated the use of the revised codes by applying them to a six-layer synthetic model 9 built on actual borehole logs; the codes are effective and convenient for joint inversion of 10 seismic data at multiple CDPs.

11 We performed comparison studies based on the synthetic six-layer model to 12 demonstrate the value of PS data for inversion of reservoir parameters. We compared the 13 inversion results obtained from using full PP stacks only, full PP stacks plus AVO 14 gradient stacks, and full PP stacks plus PS full stacks. We found that PS data are very 15 helpful for improving the estimates of porosity and floating-grain fraction and for 16 improving the estimates of effective S-wave velocity and layer-thickness under a range of 17 priors and noise levels in seismic data. Net-to-gross is relatively less sensitive to PS data. 18 Compared to the posterior results obtained from full PP plus AVO gradient stacks, we 19 found that full PP stacks are most informative for parameter estimation, then full PS 20 stacks, and finally AVO gradient stacks. This suggests that to improve the estimates of 21 reservoir parameters, full PS stacks are more valuable because PS data can provide 22 complementary information to PP full data, and give similar but better information than

- AVO gradient data. Consequently, they have the potential of significantly improving
 parameter estimation results.

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5

APPENDIX A

6 DERIVATION OF MEASUREMENT EQUATION FOR TWO-LAYER MODELS

7 Let $R_{fullPP}(0)$ be the full PP stack with the incident angle of zero and let $R_{fullPS}(\theta)$

8 and $R_{AVO-gradient}(\theta)$ be the full PS and AVO gradient stacks with the incident angle of θ .

9 From equations 6-8, we have $R_{fullPP}(0) = A_0$, $R_{fullPS}(\theta) = A_1\theta$, and $R_{AVO-gradient}(\theta) = A_2\theta^2$.

10 Let $\mathbf{R} = (R_{fullPP}(0), R_{fullPS}(\theta), R_{AVO-gradient}(\theta))^T$ be the reflectivities at the interface, where

11 T represents the transpose of a vector or matrix. Let \mathbf{R}_m be the measurements with noise

12 added, i.e., $\mathbf{R}_m = \mathbf{R} + \boldsymbol{\varepsilon}_m$. Thus, we have

13
$$\mathbf{R}_{m} = \begin{pmatrix} R_{fullPP}(0) \\ R_{fullPS}(\theta) \\ R_{AVO-gradient}(\theta) \end{pmatrix} + \boldsymbol{\varepsilon}_{m} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \theta & 0 \\ 0 & 0 & \theta^{2} \end{pmatrix} \begin{pmatrix} A_{0} \\ A_{1} \\ A_{2} \end{pmatrix} + \boldsymbol{\varepsilon}_{m} = \mathbf{M}_{\theta} \Delta \mathbf{C} + \boldsymbol{\varepsilon}_{m} .$$
(A-1)

14

APPENDIX B

15 ANGLE-DEPENDENT MATRICES FOR SYNTHETIC TWO-LAYER MODELS

16 For the case of using only full PP stacks, we set $\mathbf{M}_{\theta} = (1,0,0)$. For the case of using

17 full PP and full PS stacks, we set

$$\mathbf{M}_{\theta} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \theta & 0 \end{pmatrix}. \tag{B-1}$$

2 Similarly, for the case of using full PP and AVO gradient, we set

$$\mathbf{M}_{\theta} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \theta^2 \end{pmatrix}. \tag{B-2}$$

4 For the case of using all seismic data, we set

5
$$\mathbf{M}_{\theta} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \theta & 0 \\ 0 & 0 & \theta^2 \end{pmatrix}.$$
 (B-3)

6

1

3

APPENDIX C

7 DERIVATION OF MEAN VECTOR AND COVARIANCE MATRICES

8 In the current study, we assume the reservoir parameters under estimation are 9 loading-depth and floating-grain fraction. Let v_{pi} , v_{si} , ρ_i , z_i , and x_i be seismic P- and S-10 wave velocity, density, loading depth, and floating-grain fraction at the i-th layer, 11 respectively. From the rockphysics model in given equation 1-5, we have

12
$$\mathbf{r}_{i} = \begin{pmatrix} v_{pi} \\ v_{si} \\ \rho_{i} \end{pmatrix} = \begin{pmatrix} a_{vp} \\ a_{vs} + a_{vp}a_{vs} \\ a_{\rho} + a_{vp}b_{\rho} \end{pmatrix} + \begin{pmatrix} b_{vp} & c_{vp} \\ b_{vp}b_{vs} & c_{vp}b_{vs} \\ b_{vp}b_{\rho} & c_{vp}b_{\rho} + c_{\rho} \end{pmatrix} \begin{pmatrix} z_{i} \\ x_{i} \end{pmatrix} + \begin{pmatrix} \varepsilon_{vp} \\ b_{vs}\varepsilon_{vp} + \varepsilon_{vs} \\ b_{\rho}\varepsilon_{vp} + \varepsilon_{\rho} \end{pmatrix}$$
$$= \mathbf{\mu}_{ri} + \mathbf{H}_{i}\mathbf{\alpha}_{i} + \mathbf{\varepsilon}_{ri}.$$
 (C-1)

We can form vectors and matrices for all the layers by stacking those layer-based vectors and matrices, i.e., $\mathbf{r} = (\mathbf{r}_1^T, \mathbf{r}_2^T, \dots, \mathbf{r}_n^T)^T$, $\boldsymbol{\mu}_r = (\boldsymbol{\mu}_1^T, \boldsymbol{\mu}_2^T, \dots, \boldsymbol{\mu}_n^T)^T$, $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1^T, \boldsymbol{\alpha}_2^T, \dots, \boldsymbol{\alpha}_n^T)^T$, $\boldsymbol{\epsilon}_r = (\boldsymbol{\epsilon}_1^T, \boldsymbol{\epsilon}_2^T, \dots, \boldsymbol{\epsilon}_n^T)^T$, and $\mathbf{H} = (\mathbf{H}_1^T, \mathbf{H}_2^T, \dots, \mathbf{H}_n^T)^T$. 1 It is straightforward to derive covariance matrix from equation B-1 by assuming 2 residuals ε_{vp} , ε_{vs} , and ε_{ρ} in equations 1-3 have Gaussian distributions with zero mean 3 and variances of σ_{vp}^2 , σ_{vs}^2 , and σ_{ρ}^2 , respectively. Specifically, the matrix is

4
$$\Sigma_{ri} = \sigma_{vp}^{2} \begin{pmatrix} 1 & b_{vs} & b_{\rho} \\ b_{vs} & b_{vs}^{2} + \sigma_{vs}^{2} / \sigma_{vp}^{2} & b_{vs}b_{\rho} \\ b_{\rho} & b_{vs}b_{\rho} & b_{\rho}^{2} + \sigma_{\rho}^{2} / \sigma_{vp}^{2} \end{pmatrix}.$$
 (C-2)

5 The covariance matrix $\Sigma_r = diag(\Sigma_1, \Sigma_2, \dots, \Sigma_n)$.

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FIGURE CAPTIONS

2	Figure 1: Likelihoods of floating-grain fraction given various data combinations for the
3	true value of (a) 0.0% and (b) 3.5%. The black, green, red, and blue curves show the
4	likelihoods of using (1) full PP stacks only, (2) full PP and AVO gradient stacks, (3)
5	full PP and PS stacks, and (4) all three types of seismic data.
6	Figure 2: Likelihood ratios of using various combinations of seismic data to that of using
7	full PP stacks only as a function of measurement errors in full PS and AVO gradient
8	stacks. The green, red, and blue curves show the results of using full PP and AVO
9	gradient stacks, full PP and PS stacks, and all three data sets, respectively.
10	Figure 3: Dependent relationships among unknown parameters and data.
11	Figure 4: Various logs from an actual borehole as a function of depth: (a) P-wave
12	velocity (ft/s), (b) S-wave velocity (ft/s), (c) density (g/cc), (d) Vp/Vs, and (e) P-
13	Impedance (MPa). The solid red line segments in (a) are the approximate layer
14	interfaces.
15	Figure 5: Six-layer model, where Layers 4 and 6 are oil reservoir with oil saturation of
16	0.62, net-to-gross of 0.65, and floating-grain fraction of 0.035.
17	Figure 6: Normalized PP and PS wavelets extracted from an actual field site.
18	Figure 7: Seismic data without noise added.
19	Figure 8: Posterior probability distribution of floating-grain fraction when priors about
20	floating-grain fraction and net-to-gross are strong (i.e., $X \sim N(0.02, 0.03^2)$ and
21	$NG \sim N(0.6, 0.1^2)$, the reference case).

1	Figure 9: Posterior probability distribution of floating-grain fraction when the prior				
2	about floating-grain fraction is weak (i.e., $X \sim N(0.0, 0.05^2)$).				
3	Figure 10: Posterior probability distribution of floating-grain fraction when the prior				
4	about net-to-gross is weak (i.e., $NG \sim N(0.5, 0.3^2)$).				
5	Figure 11: Posterior probability distribution of floating-grain fraction when errors in				
6	AVO gradient and full PS stacks are doubled.				
7	Figure 12: Comparison of differences between the true values and estimated medians for				
8	priors $X \sim N(0.02, 0.03^2)$, $NG \sim N(0.5, 0.1^2)$, and noise of 0.01 for full PP and 0.02				
9	for others.				
10	Figure 13: Comparison of half-widths of 95% predictive intervals for priors				
11	$X \sim N(0.02, 0.03^2)$, $NG \sim N(0.5, 0.1^2)$, and noise of 0.01 for full PP and 0.02 for				
12	others.				
13	Figure 14: Comparison of predictive probability of the true values for priors				
14	$X \sim N(0.02, 0.03^2)$, $NG \sim N(0.5, 0.1^2)$, and noise of 0.01 for full PP and 0.02 for				
15	others.				

	Regression Equations	Standard	Units
		Errors	
0 1	$v_p = 2.12 \times 10^3 + 5.08 \times 10^{-1} Z + 1.80 \times 10^4 X$	344	ft/s
Sand	$v_s = -4.00 \times 10^3 + 8.94 \times 10^{-1} v_p$	226	ft/s
	$\rho = 1.70 + 5.04 \times 10^{-5} v_p + 1.56X$	0.0149	g/cc
<u>Q1</u> , -1 -	$v_p = (-5.38 \times 10^3) + 9.46 \times 10^{-1}Z$	476	ft/s
Snale	$v_s = -3.3730 \times 10^3 + 8.0120 \times 10^{-1} v_p$	226	ft/s
	$\rho = 0.534 v_p^{0.166}$	0.030	g/cc

 Table 1: Sand and shale rock-physics model coefficients from actual borehole logs

	Layer-1	Layer-2	Layer-3	Layer-4	Layer-5	Layer-6
Geology	Hard	Soft	Shale	Upper	Shale	Lower
	Marl	Marl		Sand		Sand
Vp (km/s)	3.67	2.85	3.32	3.49	3.48	3.58
Vs (km/s)	1.75	1.17	1.63	1.89	1.76	1.97
Density	2.54	2.38	2.50	2.39	2.52	2.41
(g/cc)						
Vp/Vs	2.10	2.44	2.04	1.84	1.98	1.81
Net-to-gross	0.0	0.0	0.0	0.65	0.0	0.65
(NG)						
Porosity				0.187		0.181
Floating-				0.035		0.035
grain fraction						

 Table 2: Synthetic six-layer model parameters

Interfaces	Full PP Stack	Angle-weighted AVO	Angle-weighted Full
	(0 degrees)	gradient Stack	PS Stack
		(45 degrees)	(45 degrees)
Layers 1 and 2	-0.159	0.135	0.328
Layers 2 and 3	0.100	-0.133	-0.272
Layers 3 and 4	0.004	-0.070	-0.088
Layers 4 and 5	0.025	0.031	0.019
Layers 5 and 6	-0.010	-0.054	-0.057

 Table 3: PP and PS reflectivities of six-layer models



Figure 1. Likelihoods of floating-grain fraction given various data combinations for the true value of (a) 0.0% and (b) 3.5%. The black, green, red, and blue curves show the likelihoods of using (1) full PP stacks only, (2) full PP and AVO gradient stacks, (3) full PP and PS stacks, and (4) all three types of seismic data.

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Figure 2. Likelihood ratios of using various combinations of seismic data to that of using full PP stacks only as a function of measurement errors in full PS and AVO gradient stacks. The green, red, and blue curves show the results of using full PP and AVO gradient stacks, full PP and PS stacks, and all three data, respectively.

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Figure 3. Dependent relationships among unknown parameters and data.



Figure 4. Various logs from an actual borehole as a function of depth: (a) P-wave velocity (ft/s), (b) S-wave velocity (ft/s), (c) density (g/cc), (d) Vp/Vs, and (e) P-Impedance (MPa). The solid red line segments in (a) are the approximate layer interfaces.

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Hard Marl
Soft Marl
Shale
Upper Sand
Shale
Lower Sand

Figure 5. Six-layer model, where layers 4 and 6 are oil reservoir with oil saturation of 0.62, net-to-gross of 0.65, and floating-grain fraction of 0.035.



Figure 6. Normalized PP and PS wavelets extracted from an actual field site.



Figure 7. Seismic data without noise added.

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Figure 8. Posterior probability distribution of floating-grain fraction when priors about floating-grain fraction and net-to-gross are strong (i.e., $X \sim N(0.02, 0.03^2)$ and $NG \sim N(0.6, 0.1^2)$, the reference case).

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Figure 9. Posterior probability distribution of floating-grain fraction when the prior about floating-grain fraction is weak (i.e., $X \sim N(0.0, 0.05^2)$).

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Figure 10. Posterior probability distribution of floating-grain fraction when the prior about net-to-gross is weak (i.e., $NG \sim N(0.5, 0.3^2)$).

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Figure 11. Posterior probability distribution of floating-grain fraction when errors in AVO gradient and full PS stacks are doubled.

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Figure 12. Comparison of differences between the true values and estimated medians for priors $X \sim N(0.02, 0.03^2, NG \sim N(0.5, 0.1^2))$, and noise of 0.01 for full PP and 0.02 for others.



Figure 13. Comparison of half-widths of %95 predictive intervals for priors $X \sim N(0.02, 0.03^2, NG \sim N(0.5, 0.1^2))$, and noise of 0.01 for full PP and 0.02 for others.



Figure 14. Comparison of predictive probability of the true values for priors $X \sim N(0.02, 0.03^2, NG \sim N(0.5, 0.1^2))$, and noise of 0.01 for full PP and 0.02 for others.