

Near-Surface Full-Waveform Inversion Reveals Bedrock Controls on Critical Zone Architecture

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Key Points:

- We perform full-waveform inversion on shallow seismic refraction data to study critical zone architecture in the Laramie Range, Wyoming.
- Borehole data confirm that the full-waveform inversion result is more accurate than conventional traveltimes tomography.
- The full-waveform inversion model reveals critical zone heterogeneity likely caused by lateral changes in bedrock properties.

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Abstract

For decades, seismic imaging methods have been used to study the critical zone, Earth's thin, life-supporting skin. The vast majority of critical zone seismic studies use travel-time tomography, which poorly resolves heterogeneity at many scales relevant to near-surface processes, therefore, limiting progress in critical zone science. Full-waveform inversion can overcome this limitation by leveraging more of the seismic waveform and enhancing the resolution of geophysical imaging. In this study, we apply full-waveform inversion to elucidate previously undetected heterogeneity in the critical zone at a well-studied catchment in the Laramie Range, Wyoming. In contrast to traveltimes tomograms from the same data set, our results show variations in depth to bedrock ranging from 5 to 60 meters over lateral scales of just tens of meters and image steep low-velocity anomalies suggesting hydrologic pathways into the deep critical zone. Our results also show that areas with thick fractured bedrock layers correspond to zones of slightly lower velocities in the deep bedrock, while zones of high bedrock velocity correspond to sharp vertical transitions from bedrock to saprolite. By corroborating these findings with borehole imagery, we hypothesize that lateral changes in bedrock fracture density majorly impact critical zone architecture. Borehole data also show that our full-waveform inversion results agree significantly better with velocity logs than previously published traveltimes tomography models. Full-waveform inversion thus appears unprecedentedly capable of imaging the spatially complex porosity structure crucial to critical zone hydrology and processes.

Plain Language Summary

Weathering processes within Earth's shallow subsurface break down rock into porous, mineral-rich materials from which biota can access water and garner nutrients. Therefore, knowledge about weathering helps scientists better understand how Earth supports terrestrial life. An effective way of studying weathering is seismic imaging, where by listening at Earth's surface to how mechanical waves propagate, we can make pictures of what is below and observe weathering in action. The seismic imaging method usually used to study weathering is first arrival traveltimes tomography which produces blurry pictures of the subsurface. We applied an advanced seismic imaging technique called full-waveform inversion, which produces higher-resolution images. Our full-waveform inversion pictures imply that changes in bedrock fracture density over relatively small lateral

50 distances have a significant effect on how weathering processes operate. When the frac-
51 ture density in the bedrock is low, there is a sharp transition from highly weathered ma-
52 terials to unaltered bedrock below. When the fracture density is high, the transition is
53 more diffuse, and there exists a thick layer of weathered bedrock. Additionally, we ground-
54 truth these interpretations with in-situ observations made in boreholes. Hence, full-waveform
55 inversion appears capable of revealing new insights into subsurface structure and weath-
56 ering processes.

57 1 Introduction

58 Nearly all terrestrial life resides in the critical zone (CZ), the volume spanning the
59 roof of vegetation down to the top of bedrock. Soil, saprolite, and weathered bedrock
60 within the CZ support terrestrial life by supplying water and nutrients to vegetation (e.g.,
61 Brantley et al., 2007; Hahm et al., 2013; McCormick et al., 2021). Weathering processes
62 are fundamental to CZ structure and function by creating porosity and permeability for
63 groundwater and by releasing nutrients from bedrock for biological uptake (e.g., Daw-
64 son et al. 2020; Hahm et al. 2019; Klos et al., 2018; McCormick et al. 2021; Meunier et
65 al., 2007; Navarre-Sitchler et al., 2015; Riebe et al., 2016). In eroding landscapes, weath-
66 ering processes sculpt a CZ architecture that generally consists of, from top to bottom,
67 soil, saprolite, weathered/fractured bedrock, and finally intact/unweathered bedrock. While
68 this layered framework is a useful starting point, CZ structure varies strongly, both within
69 and between sites (e.g., Basilevskaya et al., 2013; St. Clair et al., 2015). Understanding
70 the magnitude and scales of CZ heterogeneity requires improved knowledge of subsur-
71 face structure.

72 Because direct observations of the subsurface portion of the CZ are difficult, requir-
73 ing trenches, soil pits, or boreholes, geophysical imaging is often used to study the shal-
74 low subsurface (e.g., Parsekian et al., 2015). Seismic imaging has the advantage of be-
75 ing primarily sensitive to porosity (e.g., Callahan et al., 2020; Flinchum et al., 2018; Hayes
76 et al., 2019; Holbrook et al., 2014), which determines subsurface water storage capac-
77 ity and reflects chemical and physical weathering in eroding landscapes. In the near-surface,
78 the seismic methods most commonly used are first-arrival travelttime tomography (FATT)
79 and multichannel analysis of surface waves (MASW). These methods have been reliably
80 applied in engineering and research contexts for decades (e.g., Pasquet et al., 2016; Xia
81 et al., 1999). In particular, FATT has been used extensively to study variations in CZ

82 architecture at scales of tens of meters (e.g., Befus et al., 2011; Holbrook et al., 2014; Calla-
83 han et al., 2022; Huang et al., 2021; St. Clair et al., 2015).

84 Despite the utility of FATT and MASW methods, CZ outcrops and boreholes typ-
85 ically show much more compositional and structural heterogeneity than is captured in
86 typical seismic images. For example, borehole logs and recovered core often show small-
87 scale weathering zones, corestones, root systems, compositional variations, and fractures
88 that are not visible in smooth FATT velocity models at the same location (e.g., Flinchum
89 et al., 2022; Holbrook et al., 2019; Moravec et al., 2020). This implies that typical geo-
90 physical views of the subsurface are blurry, eliding details about CZ structure, and by
91 extension, hydrological and weathering processes. Improved resolution would enable de-
92 tection of smaller-scale heterogeneities relevant to the hydrology, biology, and geochem-
93 istry of the critical zone. Full-waveform inversion offers a means to accomplish this.

94 Full-waveform inversion (FWI) is a seismic imaging technique that can improve the
95 flexibility, fidelity, and resolution of seismic inversion by modeling the phase and/or am-
96 plitude of seismic arrivals, rather than just the arrival time. FWI is more flexible than
97 other methods because it can be applied to any part of the waveform (e.g., body waves,
98 surface waves, reflections, etc.). Fidelity is improved because FWI methods apply more
99 accurate representations of the physics governing wave propagation than, say, ray-based
100 approximations to the wave equation used in FATT or the 1D assumptions common in
101 MASW. Resolution is enhanced because FWI leverages more of the seismic waveform
102 than other methods of seismic inversion (e.g., Fichtner, 2010; Schuster, 2017). As a re-
103 sult, FWI has been widely applied in global and exploration seismology (Choi and Alkhal-
104 ifah, 2012; Lei et al., 2020; Mao et al., 2016; Pratt, 1999; Virieux and Operto, 2009). To
105 date, however, FWI has only been applied to the near surface in a handful of studies (e.g.,
106 Kohn et al., 2019; Liu et al., 2022; Sheng et al., 2006; Wang et al., 2019a, b, c).

107 Application of FWI to near-surface seismic data faces numerous challenges. First
108 is the considerable computational expense and technical overhead associated with FWI
109 as compared to FATT and MASW. Another hurdle in applying FWI is the need for domain-
110 specific inversion strategies. For example, workflows used for inverting global seismol-
111 ogy data, land seismic data, and marine reflection data all vary greatly (eg., Borisov et
112 al., 2020; Lei et al., 2020; Mao et al., 2016). FWI in the near surface is also challenging
113 because of the strong velocity contrasts and heterogeneity in elastic properties due to

114 the rapid compaction of regolith (e.g, Kohn et al., 2019; Liu et al., 2022; Sheng et al.,
115 2006). Given the limited application of FWI to study the CZ, best practices remain am-
116 biguous. A major goal of this paper is to present an FWI workflow for CZ seismic data.

117 Applications of FWI to near-surface problems to date have been aimed at a wide
118 diversity of targets, and use a variety of inversion approaches. Some studies have focused
119 on exclusively using body waves to inform shallow subsurface structure. For example,
120 Sheng et al. (2006) used first arrivals to invert for p-wave velocity (V_p) while other re-
121 searchers have used both P and S body-wave phases to constrain both V_p and shear-wave
122 velocity (V_s) (e.g., Chen et al., 2017; Liu et al., 2021). Others have primarily inverted
123 surface waves for archaeological or engineering applications (e.g., Köhn et al., 2019; Pan
124 et al., 2018; Smith et al., 2019; Wang et al., 2019c) or inverted surface waves extracted
125 from ambient noise data to study CZ structure and weathering (Wang et al., 2019a,b).
126 While this set of prior work informs how FWI can be applied in the CZ, there remain
127 several areas in which major advancements can be made. First, with the exception of
128 Wang et al. (2019a,b), all the aforementioned studies base their forward and adjoint mod-
129 eling on finite difference methods, which are not well suited to areas with complex to-
130 pography (e.g., Fichtner, 2010; Komatitsch and Vilotte, 1998). Second, nearly all pre-
131 vious applications of FWI in the CZ focused exclusively on inverting either body or sur-
132 face waves, but not both, meaning much of the available data was left unused. Third,
133 all of these past works used proprietary codes not readily available to all. Finally, those
134 prior studies were unable to ground truth their methods and results against borehole logs.

135 Our work builds on previous applications of FWI in the CZ by creating a work-
136 flow that, for the first time, combines all of the following features. First, our workflow
137 enables full elastic wave propagation across complex topography via the spectral element
138 method (e.g., Komatitsch and Tromp, 1999; Komatitsch and Vilotte, 1998). Second, our
139 FWI strategy is informed by sensitivity analyses (e.g., Tape et al., 2010) and tailored
140 to elucidate CZ structure using both surface and body waves. Third, our method is im-
141 plemented using readily available open-source packages which enable optimized compu-
142 tation via graphics cards on standard workstations (Chow et al., 2020; Komatitsch and
143 Tromp, 1999; Modrak et al., 2018). Finally, we selected a dataset with which we can test
144 our results against data from two boreholes.

145 The resulting FWI workflow is broadly applicable to the seismic refraction data sets
146 commonly acquired for CZ science. These results bring the CZ community one step closer
147 to routinely imaging subsurface CZ heterogeneity, including weathering profiles, fracture
148 zones, and corestones. In the following sections, we discuss our study site, describe our
149 FWI method and workflow, benchmark the method against synthetic data, present FWI
150 results that show remarkable heterogeneity corroborated by downhole data, and discuss
151 the implications of this work for improving our understanding of CZ processes.

152 **2 Study Site**

153 The Blair Wallis (BW) catchment is located in the Medicine Bow National For-
154 est, ~ 21 km southeast of Laramie, WY. Over the past decade, the site was studied ex-
155 tensively by the Wyoming Center for Environmental Hydrology (WyCEHG). The to-
156 pography of BW exhibits gently undulating hillslopes (Bradley, 1987; Chapin & Kelley,
157 1997; Egger et al., 1969; Evanoff, 1990). BW receives about 620 mm of annual precip-
158 itation, most of which ($> 90\%$) is snow, and has a mean annual temperature of 5.4°C
159 (Natural Resources Conservation Service, 2015). Along the ridges, sagebrush is the dom-
160 inant vegetation, while aspens, lodgepole pines, and willows appear in topographic lows.

161 BW is underlain by the Sherman Granite, a sub-unit of the 1.4 GA Sherman Batholith
162 that was uplifted during the Laramide Orogeny (Frost et al., 1999; Peterman & Hedge,
163 1968; Zielinski et al., 1982). The mineralogical makeup of the coarse-grained Sherman
164 Granite is roughly 40-55 % potassium feldspar, 15 – 30 % quartz, 20 % plagioclase feldspar,
165 and 5 – 10 % biotite (Edwards & Frost, 2000; Frost et al., 1999; Geist et al., 1989). While
166 there is no recognizable metamorphic fabric in the rock, a pervasive tectonically induced
167 NE-SW striking fracture population can be observed in outcrops and in aerial imagery.
168 These fractures dip $30 - 80^\circ$ and cause the bedrock and saprolite to exhibit moderate
169 seismic anisotropy (Novitsky et al., 2018).

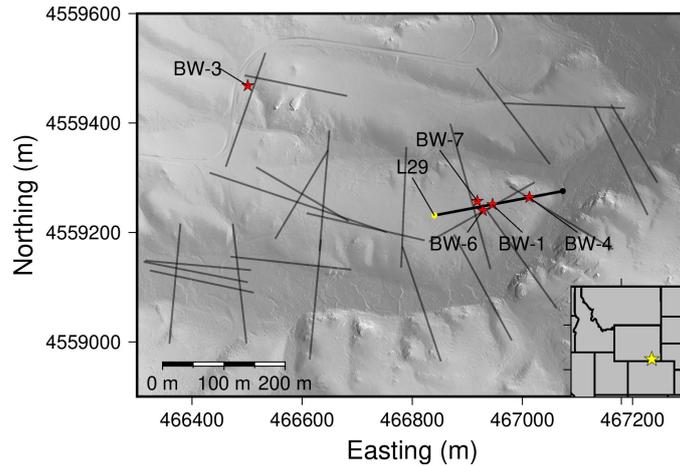


Figure 1. Hill shade map of the BW study site taken from Flinchum et al. (2022), where various seismic refraction profiles collected by WyCEHG are demarcated with black lines. The seismic refraction profile used in this study is L29. The yellow dot indicates where $x = 0$ along the transect. The red stars show the locations of boreholes that were drilled and logged. In this work, we show borehole logs from BW1 and BW4 which are located directly on L29.

170 3 Methods

171 In July 2013, WyCEHG collected a 239-m-long seismic refraction line along a ridge
 172 in BW (Figure 1). First arrival traveltimes of these data were manually picked, inverted
 173 using FATT, and published first in Flinchum et al. (2018) and later in Flinchum et al.
 174 (2022). Our workflow followed these steps, each of which is described in more detail in
 175 sections 3.2-3.5 below. First we used the Flinchum et al. (2022) V_p model as the start-
 176 ing V_p model and to estimate source time functions. Second, we constructed an initial
 177 V_s model using wave equation dispersion inversion (e.g., Li et al., 2016). Third, we con-
 178 ducted sensitivity analysis of the phases we inverted using the adjoint state method (e.g.,
 179 Tromp et al., 2005). Finally, we applied FWI to the data using a custom workflow tai-
 180 lored to the challenges of near-surface seismic data.

181 3.1 Seismic Data

182 Data used in this study were acquired on a linear array of 240 vertical-component
 183 geophones spaced at 1 m intervals and sampled every 500 μ s over a record length of 1
 184 s. The frequency response of the geophones increases from 0 – 4.5 Hz and then is vir-

185 tually flat up to 1,000 Hz. A total of 20 sledgehammer source points generated seismic
 186 energy every 12 m along the profile, with one missing source at 24 m.

187 The recorded waveforms show multiple distinct phases, including first arrival p-waves,
 188 a p-wave coda phase directly behind the first arrival, a clear fundamental mode Rayleigh
 189 wave phase, and a higher-mode surface wave. The body wave phases display a broader
 190 bandwidth with more energy at higher frequencies (8 - 56 Hz), while the surface waves
 191 exhibit narrower bands concentrated around lower frequencies (6 - 22 Hz) (Figure 2). In
 192 section 3.4 we perform sensitivity analysis on each of the four phases identified in the
 193 top right panel of Figure 2.

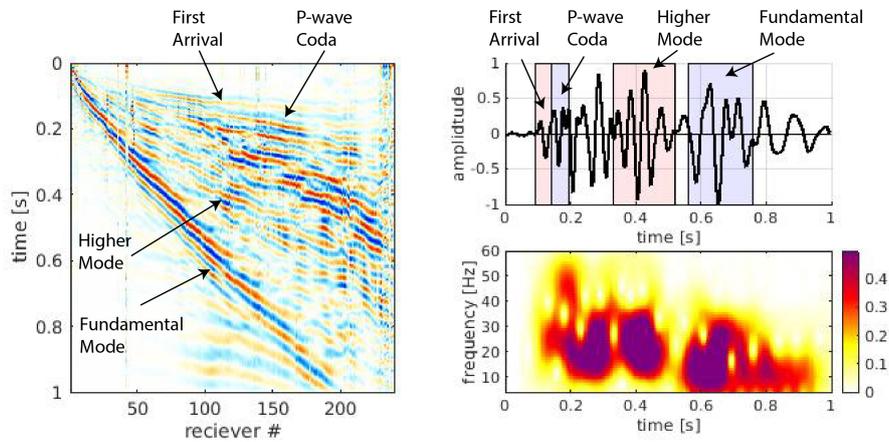


Figure 2. Left panel: a filtered (5-56 Hz) shot gather from a source located 0 m along the transect. Upper right panel: the geophone recording for the instrument located 120 m along the transect. The first arrival, p-wave coda, higher mode surface wave, and fundamental mode surface wave are highlighted. Each waveform in the highlighted boxes is back-projected to construct the sensitivity kernels in Figure 4. Bottom right panel: a spectrogram of the trace in the upper right panel, showing higher frequencies in the P-wave first arrival and lower frequencies in the Rayleigh wave.

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3.2 Source Estimation

Because the source time function (STF) at each hammer location may vary depending on local ground conditions, the individual generating the source, and potentially other

factors (Figure S1), it is necessary to estimate a unique STF at each source location. Because our initial FATT Vp model accurately predicts first arrival times, it is suitable for estimating the STF for each shotpoint, using (e.g., Borisov et al., 2020; Pratt, 1999):

$$s(\omega) = \sum_{i \in \text{window}} \frac{u_i^0(\omega) \cdot g_i^*(\omega)}{g_i(\omega) \cdot g_i^*(\omega) + \gamma} \quad (1)$$

195 In equation (1), i is the index of a particular trace, u^0 is preprocessed observed data, g
 196 is preprocessed data modeled using a STF with a unit frequency spectrum, $*$ denotes
 197 the complex conjugate, γ is a regularization parameter which also helps avoid division
 198 by zero, and s is the estimated STF. For the source estimation, the preprocessing steps
 199 include normalizing the waveforms such that the maximum amplitude of each trace is
 200 1 and muting out everything except the first arrivals by applying a time window behind
 201 the first arrival pick with a duration of $1/f_0$ where $f_0 = 30$ Hz is roughly the dominant
 202 frequency of the data. We only use first arrivals to inform the STF estimates because
 203 these are the only phases reliably fit by the FATT model. To minimize near-source ef-
 204 fects and to boost signal/noise ratios, we stacked data over offsets of 100 – 175 m. Us-
 205 ing data at these offsets to inform the STF also helps account for some of the unmod-
 206 elled effects of anelastic attenuation (e.g., Borisov et al., 2020).

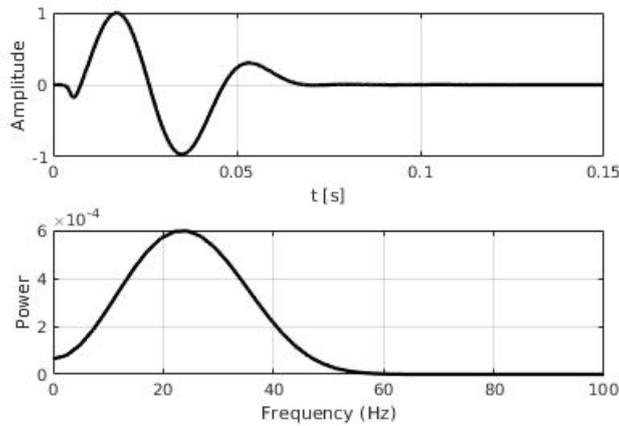


Figure 3. The estimated source time function and frequency spectrum for the hammer swing located at $x = 0$ m.

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3.3 Initial Shear-Wave Velocity Model

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With an estimate of the STFs in hand, next we built a suitable starting Vs model for FWI. Rather than using a scaled version of the starting Vp model for this purpose (e.g., Liu et al., 2022), we found that a more rigorous prior estimate of the Vs field is necessary to perform FWI on the surface waves. To do this, we leveraged the well-known phenomenon of surface wave dispersion using the wave equation dispersion inversion (WD) technique developed by Li et al. (2016). WD is a skeletonized data inversion strategy, meaning that it uses the same forward and adjoint modeling typically employed in FWI, but fits a significantly smaller portion of the data. While this results in a lower resolution inversion, unlike FWI, the convergence of WD is almost guaranteed.

The WD method minimizes the following functional

$$\chi^{WD} = \frac{1}{2} \sum_{i=1}^{N_s} \int_{\omega} \Delta\kappa_i(\omega)^2 d\omega \quad (2)$$

where i is the source index, N_s is the number of sources, ω is the angular frequency, and $\Delta\kappa$ is the difference between the dispersion curves of observed and synthetic data. To compute $\Delta\kappa$, two Fourier transforms are performed on the preprocessed synthetic and observed shot gathers, $U(t, x)$ and $U^0(t, x)$, to derive $\tilde{U}(\omega, \kappa)$ and $\tilde{U}^0(\omega, \kappa)$ respectively, transforming the shot gathers from the time-offset domain to the angular frequency-wavenumber domain. Then, for each ω , $\Delta\kappa$ is calculated via cross-correlation such that

$$\Delta\kappa(\omega) = \arg \max_{\kappa} \mathcal{R} \left\{ \int \tilde{U}(\omega, \kappa') \cdot \tilde{U}^0(\omega, \kappa' + \kappa) d\kappa' \right\}, \quad (3)$$

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with $\mathcal{R}\{\cdot\}$ taking the real part of a complex number. The preprocessing during the WD inversion involves normalizing all traces and muting data outside the 10 - 75 m offset range. The shear-wave velocity of the starting model for the WD inversion increases linearly with depth. Due to the limited depth sensitivity of the WD method, the lower portion of the final WD model is altered to be a scaled version of the FATT Vp model by a factor of two.

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3.4 Sensitivity Analysis

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With an initial model parameterized, we can compute the traveltime sensitivity kernels (also known as banana-doughnut kernels or Fréchet Derivatives) of the four read-

226 ily identifiable phases: the first arrival, p-wave coda, higher mode surface wave, and fun-
227 damental mode surface wave (Figure 2). For demonstration purposes, we used the trace
228 and windows shown in the upper right panel of Figure 2 to back project the time-reversed
229 particle velocity at the receiver location through the initial model (e.g., Tromp et al., 2005;
230 Fichtner et al., 2008; Tape et al., 2010) (Figure 4). Repeating this sensitivity analysis
231 on other source-receiver pairs yielded similar results. The sensitivity analysis is an im-
232 portant step in our workflow as it provides insights into which waveforms are useful for
233 updating certain model parameters.

234 For example, the traveltime kernel of the first arrival is characteristic of a diving
235 wave, exhibiting the quintessential banana shape often associated with teleseismic body
236 waves in vertical cross-section (top left panel of Figure 4). Along the ray path, the ker-
237 nel is negative, meaning that a decrease in the wave speed will result in an increase in
238 traveltime (e.g., Tromp et al., 2005). The traveltime kernel of the first arrival has a wide
239 sensitivity zone, indicating a broad depth range determines the diving wave arrival time.
240 The p-wave coda, in contrast, appears to travel primarily in the near-surface and is sen-
241 sitive to a narrower depth range (second row of Figure 4). Regardless of the paths the
242 energy takes, both types of body waves are primarily sensitive to V_p (Figure 4). The fun-
243 damental mode Rayleigh wave traveltime is primarily sensitive to the upper 15 – 20 m,
244 while the higher mode Rayleigh wave shows a more complicated sensitivity kernel, with
245 deeper and shallower sensitivity where energy focuses and defocuses respectively (third
246 and last rows Figure 4 respectively). Although other clear phases exist in the vertical-
247 component data (Figure 2), we were unable to use sensitivity analysis to confirm that
248 any of these arrivals are shear or converted body waves. However, our method is appli-
249 cable to such phases if observed.

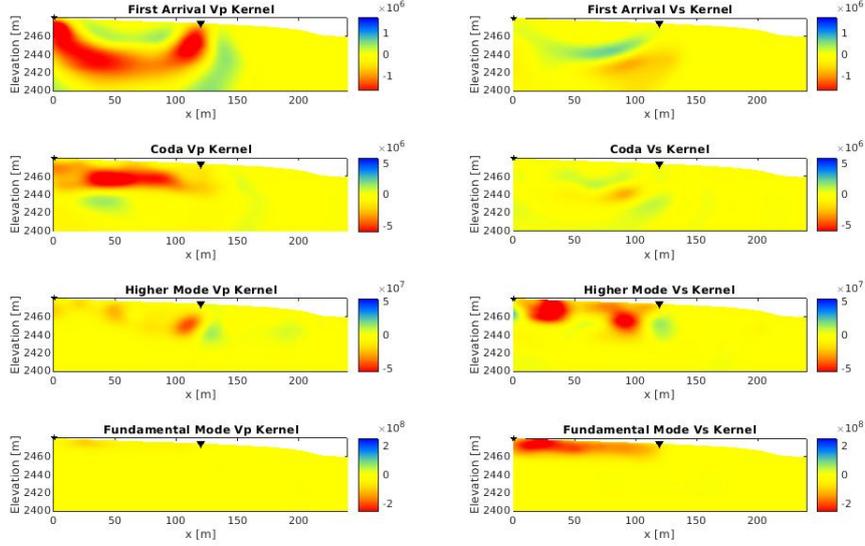


Figure 4. Sensitivity kernels with respect to each model parameter (V_p and V_s) for each of the four highlighted phases in the upper right panel of Figure 2. The first column corresponds to sensitivity with respect to V_p , while the second column corresponds to sensitivity with respect to V_s . The first row shows the sensitivity of the first arrival, the second row shows the sensitivity of the p-wave coda, the third row shows the sensitivity of the higher mode surface wave, and the last row shows the sensitivity of the fundamental mode surface wave.

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3.5 Full-Waveform Inversion Workflow

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In this study, we used a fork of the FWI workflow manager SeisFlows published by Modrak et al. (2018), which primarily serves as a wrapper for the forward and adjoint (an)elastic wavefield solver, *specfem2d* (Komatitsch and Tromp; 1999). The use of the spectral element method in this study is particularly important given the topographic variation in the ground surface of our model. Specifically, the free surface boundary condition at the ground surface is rigorously fulfilled by the spectral element method, unlike in other modeling strategies, such as grid-based finite difference methods (e.g., Fichtner, 2010).

During the FWI portion of our workflow, we defined the functional to be minimized, χ , using the normalized correlative (NC) misfit norm,

$$\chi = \frac{1}{N_s \cdot N_r} \sum_{i=1}^{N_s} \sum_{j=1}^{N_r} \left[1 - \int_T \hat{u}_{i,j} \cdot \hat{u}_{i,j}^0 dt \right], \quad (4)$$

where \hat{u} and \hat{u}^0 are synthetic and observed waveforms with their maximum amplitudes normalized to 1, N_s is the number of sources, and N_r is the number of receivers. $\int_T \hat{u}_{i,j} \cdot \hat{u}_{i,j}^0 dt$ is called the correlation coefficient and measures the similarity of two time series. We chose the NC norm because it is both noise-resistant and emphasizes fitting phase rather than amplitude (e.g., Borisov et al., 2020; Choi and Alkhalifah, 2012). This helps contend with noise in the data as well as certain unmodelled anelastic and 3D effects (e.g., Borisov et al., 2020). To minimize the NC norm, we iteratively update the velocity model, \mathbf{m} , according to

$$\mathbf{m}^{i+1} = -\alpha \mathbf{P} \mathbf{H} \nabla_{\mathbf{m}} \chi + \mathbf{m}^i \quad (5)$$

In the above equation, $\nabla_{\mathbf{m}} \chi$, the gradient with respect to the misfit functional, χ , is computed via the adjoint method, α is a step length computed via a bracket line search, and \mathbf{P} is a diagonal preconditioning matrix containing the discretized field P_1^{-1} which is defined as

$$P_1(x, z) := \sum_{i=1}^{N_s} \int_T \partial_t^2 u_i(x, z) \cdot \partial_t^2 u_i(x, z) dt \quad (6)$$

259 where $u_i(x, z)$ is the synthetic wavefield excited by the i th STF. The main purpose of
 260 the preconditioner is to remove numerical artifacts caused by large amplitudes near the
 261 ground surface and to account for the geometric spreading of the wavefield. In equation
 262 5, \mathbf{H} is the Hessian matrix; in practice, we approximate the Hessian-gradient product,
 263 $\mathbf{H} \nabla_{\mathbf{m}} \chi$, using a limited-memory Broyden–Fletcher–Goldfarb–Shanno algorithm (Liu and
 264 Nocedal, 1989). We used the same modeling strategy and optimization framework for
 265 the WD step of our workflow.

266 The FWI strategy used in this study was informed by our preliminary analysis of
 267 the data. We inverted surface waves and body waves separately, in different steps of the
 268 workflow, because the sensitivity with respect to surface waves is about two orders of
 269 magnitude higher than the sensitivity with respect to body waves (Figure 4). Hence it
 270 would require extreme scaling of the body waves to balance their contributions to model
 271 updates with those of the surface waves, which creates numerical artifacts. Separating

272 the surface and body waves is also advantageous because of their different frequency con-
 273 tents. Using a multiscale approach (e.g, Bunks et al., 1994; Chen et al., 2019), we work
 274 through the frequency content of the surface waves gradually, focusing on their lower fre-
 275 quencies, while we step through frequencies of the body waves more aggressively to cover
 276 their wider bandwidth.

277 With these issues in mind, we chose to invert the surface waves first, using them
 278 to inform the upper portion of the earth model. Then, in a quasi-layer-stripping approach,
 279 we updated the deeper part of the model using the body waves. During the surface wave
 280 step of the workflow, both V_p and V_s are updated, while only V_p is updated during the
 281 body wave step because the first arrivals and p-wave coda are primarily sensitive to V_p
 282 (Figure 4). We found that any V_s sensitivity shown in computed Fréchet derivatives for
 283 the first arrival or p-wave coda is likely a numerical artifact that degrades the fit of sur-
 284 face waves if incorporated into the model updates derived from the body waves (Figure
 285 4).

286 The preprocessing of waveforms in both steps included muting traces outside a parti-
 287 cular offset range, bandpass filtering, normalizing all traces to a maximum amplitude
 288 of 1, and muting various arrivals. In the surface wave inversion step, traces between 10
 289 – 150 m offset were used, with 6 – 14, 6 – 18, and 6 – 22 Hz bandpass filters applied, while
 290 all phases arriving earlier than the higher mode were muted. In the body wave step, traces
 291 between 50 – 210 m offset were used, with 8 – 24, 8 – 40, and 8 – 56 Hz bandpass fil-
 292 ters applied, and all phases arriving later than the p-wave coda were muted. To regu-
 293 larize the inversions, we smoothed the gradients by convolving them with a 2D Gaus-
 294 sian function. In the surface wave step, we used a smoothing radius of 10 m for all stages
 295 of the multiscale strategy, while for the body wave step, we used smoothing radii of 40,
 296 20, and 10 m, decreasing the smoothing radius as we increased the frequency content dur-
 297 ing each stage of the multiscale strategy.

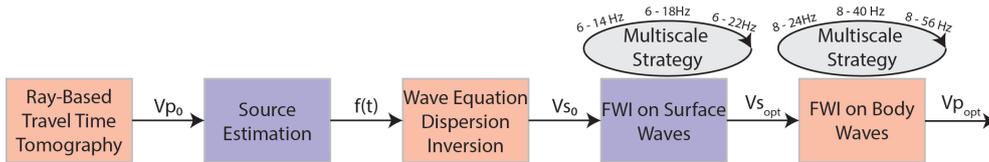


Figure 5. A flow chart of our FWI strategy showing both preliminary steps and FWI stages.

4 Results

4.1 Workflow Validation with Synthetic Data

We benchmarked the FWI portion of our workflow (the last two boxes in Figure 5) by inverting synthetic data to illustrate the kinds of features that can be recovered. For this synthetic test, we used the same survey geometry and starting Vs and Vp models as in our real data case, but added three velocity anomalies: a shallow high-velocity anomaly representing a corestone, a deeper high-velocity anomaly indicative of an area of bedrock with low fracture density, and a low-velocity zone characteristic of a fracture zone. Generally speaking, our FWI workflow recovers all three anomalies fairly well, although the shape of anomalies in the final models is not perfect (Figure 6). Nonetheless, this synthetic test bolsters confidence that we can trust relatively large-scale features (on the order of 10 m or larger) in our FWI results.

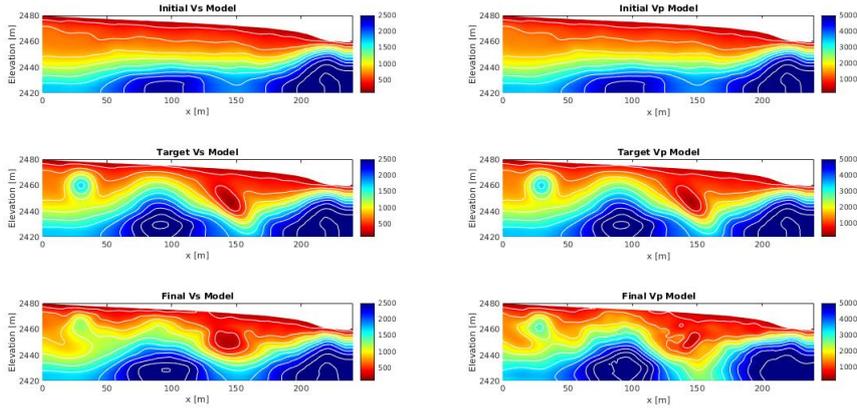


Figure 6. Results from the synthetic FWI experiment. The left column has Vs models and the right column has Vp models. The first row shows the starting models, the second row shows the target models, and last row shows the inverted models. Velocity contours on the Vs and Vp models have intervals of 250 m/s and 500 m/s respectively.

4.2 Surface Wave Step

After the FATT, source estimation, and WD, the low-frequency (6 – 14 Hz) surface wave data tends to fit within one wavelength but is not yet perfectly recovered (Fig-

313 ure S2). By the end of the first stage of the surface wave inversion, the phase informa-
 314 tion of Rayleigh waves is well represented by synthetics (Figures 7 and S2). In the lat-
 315 ter two stages, higher frequency data is progressively fit (6 – 18 Hz and 6 – 22 Hz). In
 316 these stages, only relatively small adjustments to the synthetic waveforms are needed
 317 to improve the model fits (Figures 7, S3, and S4). Generally speaking, as the frequency
 318 content of the data being fit increases, diminishing returns in decreasing the misfit func-
 319 tion are made (Figure 7).

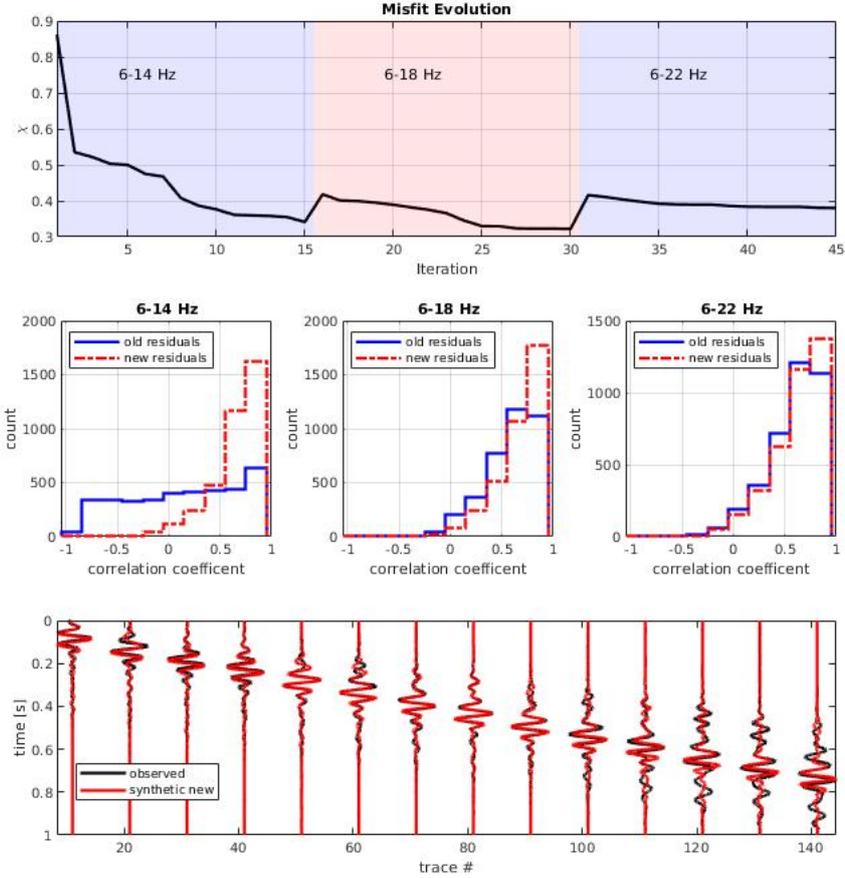


Figure 7. Top panel: The evolution of the misfit function with each FWI iteration, segmented by each stage of the multiscale strategy. Middle panels: histograms of the the correlation coefficients, $\int_T \hat{u} \hat{u}^0 dt$, for all traces before and after each stage of the multiscale strategy. Bottom panel: Preprocessed (body waves are muted and 6 - 22 Hz bandpass filtered) waveforms after surface wave FWI.

320 In the resultant Vs model, we observe several features indicative of the increased
 321 resolution gained by performing FWI using surface waves (Figure 8). One such feature
 322 is a high-velocity zone around $x = 50$ m, where the 400 – 600 m/s velocity contours are
 323 bowed upward. The strongest vertical velocity gradients occur towards the far end of the
 324 line ($x = 210 - 239$ m). Note that the casing depths of the two boreholes correspond with
 325 shear-wave velocities of 400 - 500 m/s, suggesting that these velocities may be a good
 326 range to use for inferring the boundary between saprolite and fractured bedrock.

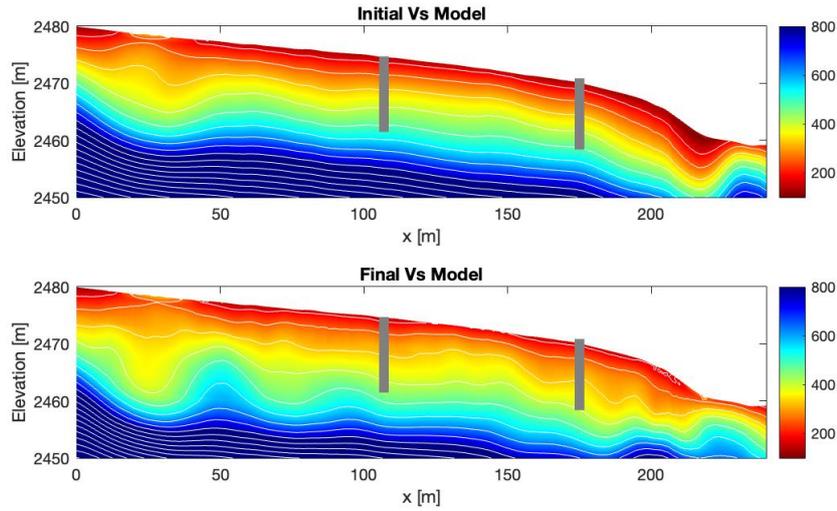


Figure 8. Shear-wave velocity models before and after FWI. Velocity contours at 75 m/s intervals are also shown in white. The gray rectangles show the locations of borehole casings. Please note the limited elevation range of these plots.

327 4.3 Body Wave Step

328 At the onset of the first stage of the multiscale strategy for the body waves, the
 329 low-frequency (8 – 24 Hz) data tends to fit reasonably well, implying that the FATT model
 330 and STF estimates provide a good initial parameterization for performing FWI (Figure
 331 S5). In the ensuing stages of the multiscale strategy, we see that both the p-wave coda
 332 and first arrival are accurately fit by the synthetics, although the data fit degrades slightly
 333 at offsets greater than 200 m (Figures 9, S5, S6, and S7). Convergence was slower for
 334 the body waves and required more iterations than during the surface wave step (Figure
 335 9).

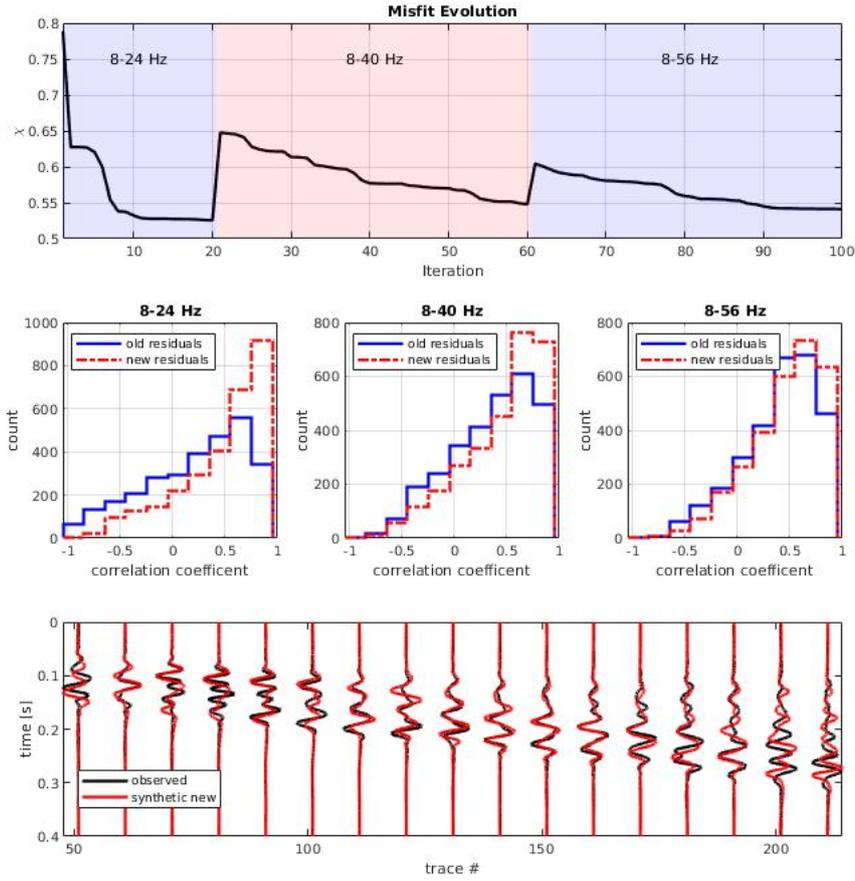


Figure 9. Top panel: The evolution of the misfit function with each FWI iteration, segmented by each stage of the multiscale strategy. Middle panels: histograms of the the correlation coefficients, $\int_T \hat{u}\hat{u}^0 dt$, for all traces before and after each stage of the multiscale strategy. Bottom panel: Preprocessed (surface waves are muted and 8 - 56 Hz bandpass filtered) waveforms after body wave FWI.

336 In the final Vp model, large updates can be observed, showing the impact of ap-
 337 plying FWI to the body waves (Figure 10). Several novel features are observed in the
 338 final Vp model, including a high-velocity zone located at around 100 m, deep low-velocity
 339 zones located around $x = 20$ and 190 m, and various fine structures in the near-surface.
 340 Generally speaking, vertical and lateral velocity gradients have increased substantially
 341 in several areas. Interestingly, there appears to be more near-surface heterogeneity in

342 the final Vp model than in the Vs model, and we discuss why this may be the case in
 343 section 5.1. Several of the features we have noted were also observed by Wang et al. (2019b),
 344 including deep low-velocity zones and more heterogeneity in Vp relative to Vs.

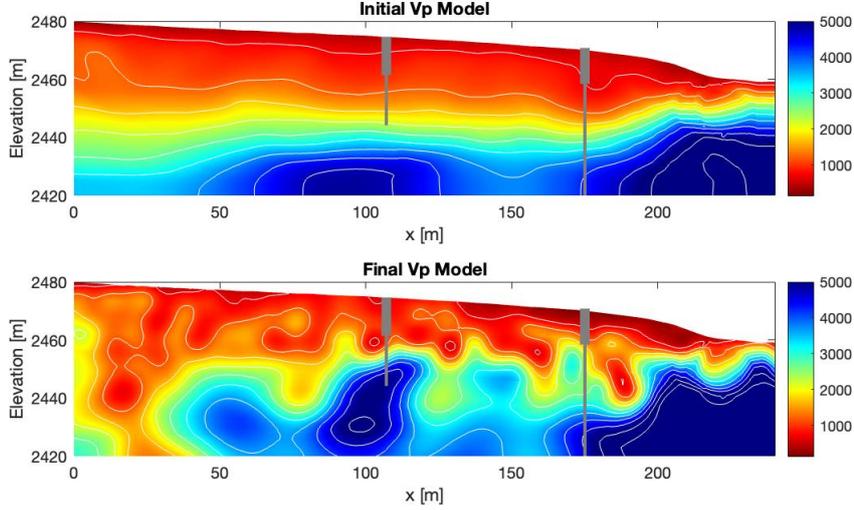


Figure 10. P-wave velocity models before and after FWI. Velocity contours at 500 m/s intervals are also shown in white. The gray rectangles show the locations of borehole casings, while the gray lines show where the borholes were logged.

345 4.4 Comparison to Borehole Data

346 Two boreholes on our profile, BW1 and BW4, located at roughly $x = 107$ and 175
 347 m, provide an opportunity to ground-truth our FWI results. As summarized in Flinchum
 348 et al. (2022), the upper parts of the boreholes drilled through incompetent soil and sapro-
 349 lite were cased, and the deeper open holes were logged. Since no borehole data from the
 350 saprolite and soil exist, we cannot compare borehole logs with the surface wave Vs mod-
 351 els where only the upper ≈ 20 m or so are constrained (Figure 4). The borehole logs
 352 are, however, an effective ground truth for the Vp models, where the diving wave pro-
 353 vides information on deep CZ structure (Figure 4).

354 The final Vp model shows much better agreement with the borehole logs than the
 355 initial model, demonstrating substantial gains from FWI (Figure 11). While the initial
 356 model created using FATT is far too smooth and incorrectly estimates velocities at mod-
 357 erate depth (15 – 30 m), after applying FWI, this inconsistency is greatly reduced. This

358 comparison suggests that FATT may underestimate vertical velocity gradients in the CZ
 359 (Figures 10 and 11). The borehole comparison suggests that both the high-velocity and
 360 low-velocity zones in our final Vp model are true features rather than inversion artifacts.
 361 Although these low-velocity zones have not been directly observed in either borehole pre-
 362 sented, the aforementioned synthetic tests support that we can recover such features us-
 363 ing our FWI workflow.

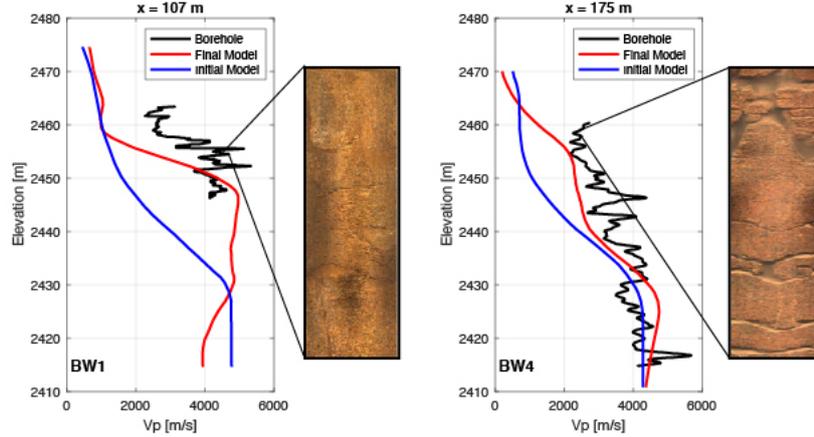


Figure 11. Comparison of the FATT and FWI Vp models with the borehole logs from BW1 (left) and BW4 (right) and expanded views of the bedrock observed in optical logs over a 2 m depth range in each hole. Note higher fracture density visible in BW-4, which corresponds to lower P-velocities in that hole.

364 5 Discussion

365 5.1 Limitations, Uncertainties, and Outlook on Future Work

366 While our results are promising, some areas of improvement exist for our method-
 367 ology, including potentially incorporating 3D modeling to more accurately recover ge-
 368 ometric wavefield spreading. While more rigorous, incorporating 3D modeling would likely
 369 require a supercomputing cluster (e.g., Chow et al., 2020; Wang et al., 2019a; Wang et
 370 al., 2019b), whereas limiting the technical overhead of FWI by implementing it on a work-
 371 station, as we have, makes the method accessible to more researchers. Furthermore, given
 372 our exclusive use of phase information and focus on inverting for velocity, incorporat-
 373 ing 3D modeling may not significantly change our results. It is more likely that the biggest

374 gains achieved by incorporating 3D modeling would also require full 3D data coverage
375 (Górszczyk et al., 2023), allowing us to recover the true 3D structure of Earth’s CZ. For
376 these reasons, we leave 3D modeling for future work.

377 Other areas of improvement for our workflow pertain to our parameterization of
378 the Earth model. For example, including a reasonable estimate of anelasticity may help
379 limit inversion artifacts (e.g., Borisov et al., 2020; Groos et al., 2014). In particular, we
380 expect anelasticity to affect the surface wave inversion to a greater extent than it would
381 the body wave inversion, as the surface waves travel significantly more cycles than the
382 body waves. Nonetheless, given the complexities of parameterizing or inverting for a dy-
383 namic and heterogeneous near-surface anelasticity field (Askan et al., 2007), we leave this
384 issue for future work. We also do not rigorously parameterize or invert for density in our
385 workflow. In our modeling, density is set as an arbitrary scalar so that Vp and Vs fields
386 can be converted to Lamé parameters for input into `specfem2d`. Changes in our param-
387 eterization of the density field could affect the amplitudes of synthetic waveforms (e.g.,
388 Liu et al., 2022). However, since we exclusively use phase information in our inversion
389 and normalize all the traces, changes in our representation of density should have little
390 to no effect on our final results. Given the inconsistent coupling of instruments in the
391 data set we used, attempting to use amplitude information to constrain density would
392 likely be ill-conceived, although future advances in instrumentation may someday make
393 this a worthwhile pursuit (e.g., Yuan et al., 2015). Additionally, since CZ materials may
394 exhibit significant seismic anisotropy (Eppinger et al., 2021; Novitsky et al., 2018), ac-
395 counting for anisotropy may further improve FWI results, although this would likely re-
396 quire some prior information about the anisotropy of the study site or 3D, multi-component
397 data coverage (e.g., Toyokuni and Zhao, 2021).

398 Another limitation in our FWI models relates to what extent the separately inverted
399 Vp and Vs fields can be used to calculate Poisson’s ratio in the CZ, given that the Vp
400 FWI model is significantly more heterogeneous than the Vs model (Figures 8 and 10).
401 It is possible that the contrast in Vp vs. Vs heterogeneity is caused by variations in the
402 fluid content of the pore spaces, since shear velocity is insensitive to water saturation.
403 Another possible explanation is that the information contained in the surface waves varies
404 from that of the body waves. Considering that anelasticity usually correlates with ve-
405 locity (e.g., Asian et al., 2007; Borisov et al., 2020), the surface waves traveling primar-
406 ily through lower-velocity material likely attenuate more than the body waves. This would

407 result in the surface waves having a lower frequency content (e.g., Figure 2) and may cause
408 models derived with them to lack high-wavenumber information. Alternatively, the Vp
409 model may contain excess heterogeneity, namely inversion artifacts caused by the lower
410 signal-to-noise ratio of the body waves. We think it would be constructive for future work
411 to investigate which of these possible explanations is most plausible.

412 Future work could also make various theoretical advancements to our FWI work-
413 flow. For example, using source encoding could significantly reduce the computational
414 cost of FWI in the CZ or reserve computational resources for incorporating 3D model-
415 ing and more data into workflows (e.g., Tromp and Bachman, 2019). More investigation
416 into which misfit function is best for FWI in the CZ would be beneficial. Looking into
417 measurements that limit errors associated with source estimation and instrument response
418 while simultaneously increasing resolution, such as the double difference measurement
419 (e.g., Yuan et al., 2016) would be worthwhile. Trialing other misfit functions that cap-
420 ture traveltimes differences of multiple events, such as the local traveltimes inversion method
421 proposed by Hu et al., (2020) could also be advantageous. Another promising branch of
422 research is uncertainty quantification for FWI in the CZ, as these methods may help re-
423 searchers to identify and avoid interpreting inversion artifacts (e.g., Thurin et al., 2019).

424 **5.2 Implications for Critical Zone Heterogeneity**

425 One of the primary challenges in capturing and characterizing critical zone processes
426 is the vast range in scales they span. At the smallest scales, chemical weathering occurs
427 at the molecular and grain scale, driven by chemical reactions on individual mineral sur-
428 faces, often aided by symbiotic fungi at the micron scale (e.g., Brantley et al., 2017; Navarre-
429 Sitchler et al., 2015; Sak et al., 2010). At larger scales, we might expect weathering to
430 depend on climatic patterns that can vary at regional or watershed scales (e.g., Good-
431 fellow et al., 2013). Other processes might be relevant at intermediate scales, including
432 compositional heterogeneity, fracture zones, slope-aspect contrasts, or bedrock foliation
433 (Callahan et al., 2022; Eppinger et al., 2021; Leone et al., 2020; Novitsky et al., 2018;
434 West et al., 2019). This diverse set of processes acting across multiple scales creates het-
435 erogeneity in subsurface CZ structure, which is visible in outcrops (e.g., Dethier and Lazarus,
436 2006), corestones (Sak et al., 2010), and thin sections (e.g., Holbrook et al., 2019). Cap-
437 turing such heterogeneity in the subsurface critical zone is a formidable challenge, for
438 which improved geophysical methods like FWI are needed.

439 Our results show that critical zone structure is laterally heterogeneous at scales much
440 smaller than can be attributed to large-scale forcing functions like climate or tectonic
441 stress. For example, the depth at which fast velocities associated with intact bedrock (V_p
442 $> \sim 4000$ m/s) is reached varies by more than a factor of two over only 15 m horizon-
443 tal distance, from ~ 20 m at $x = 110$ m to greater than 50 m at $x = 125$ m (Fig. 10).
444 Over that same stretch, the thickness of the weathered bedrock layer ($1,200$ m/s $< V_p$
445 $< 4,000$ m/s) goes from only a few meters to more than 25 m. Contrasts at this hori-
446 zontal scale cannot be the consequence of differing climate, and given the location of this
447 profile along a ridgeline, it is similarly difficult to imagine other top-down processes (e.g.,
448 hydrology, vegetation) could produce such variability. Instead, we must seek bottom-up
449 explanations for these changes, sourced in the local geology (e.g., composition or frac-
450 tures).

451 Both the boreholes and the details of the FWI inversion provide clues as to the causes
452 of these strong lateral contrasts in critical zone structure. In particular, the drilling re-
453 sults at BW1 and BW4 combined with the FWI velocity model tell a story of two dis-
454 tinct weathering fronts at these locations. At BW1, we observe strong vertical velocity
455 gradients in both the borehole log and FWI model and very few open fractures in the
456 underlying bedrock (Figure 11). Meanwhile, at BW4, the vertical velocity gradients in
457 the borehole log and FWI model are more diffuse, and more intensely fractured bedrock
458 exists at depth. These results imply that the sharpness of the transition from weathered
459 to unweathered materials depends on the fracture density of bedrock as it enters the CZ
460 weathering engine. Indeed, the thickness of the fractured bedrock layer appears to be
461 inversely correlated with the velocity of the underlying bedrock. In parts of the model
462 with very fast ($> 4,500$ m/s) bedrock velocities, there is a rapid transition to overlying
463 saprolite, with little (or no?) weathered bedrock, while elsewhere slower deep bedrock
464 underlies thick weathered bedrock layers – suggesting a bottom-up control on CZ archi-
465 tecture here (Figure 10). Such bottom-up controls could include lateral changes in com-
466 position (e.g., Brantley et al., 2017; Basilevskaya et al., 2013), foliation (Leone et al., 2020),
467 or fracture density (e.g., Novitsky et al., 2018). At our site, we suggest that changes in
468 bedrock fracture density are most likely, given the observation of fracture zones in ad-
469 jacent outcrops.

470 Additional intriguing features in the FWI model include narrow, steeply dipping
471 zones of very low velocity ($< 1,000$ m/s) that penetrate tens of meters into the subsur-

472 face at several places along the line (e.g., at $x \approx 25$ m and $x \approx 185$ m). These features
473 might represent deep zones of intense chemical weathering and fracturing. While our bore-
474 holes were not placed to verify the presence of these features, such low-velocity zones might
475 well play an outsized role in guiding water through the subsurface. Thus, full-waveform
476 inversion promises to yield important new insights into catchment hydrology.

477 Given that the full waveform results show such heterogeneity, does this imply that
478 the ray-based tomograms that have been the primary seismic tool for imaging the crit-
479 ical zone are wrong? To address this, we compared our FWI results with the FATT ini-
480 tial model. At a glance, the FWI model is much more detailed and heterogeneous than
481 the FATT model (Figure 10). A comparison of the depth ranges of velocities associated
482 with the saprolite-bedrock transition (1.2 km/s), however, reveals that while the depths
483 distributions are more variable in the FWI model, the average saprolite thicknesses are
484 similar in the FWI and FATT results (Figure 12). The same can be said for the depth
485 to intact bedrock (Figure 12). Thus, FATT accurately captures long-wavelength features
486 in the CZ but misses smaller-scale heterogeneity. That is to say, FATT models aren't wrong,
487 but they are blurry. This point is further emphasized by the upper left panel of Figure
488 4, showing the banana-doughnut kernel for the first arrival. The large volume of the ker-
489 nel implies that first arrival traveltimes are sensitive to the average velocity of a signif-
490 icant portion of the subsurface, and this detail is reflected in the blurriness of FATT mod-
491 els. These findings help contextualize previous conclusions based on FATT models, which
492 have elucidated large-scale, first-order controls on CZ structure such as slope aspect (Be-
493 fus et al., 2011), regional tectonic stresses (St. Clair et al., 2015), and foliation (Leone
494 et al., 2020). Our findings show that FWI can build on this past research by unearthing
495 the effects of smaller-scale processes. In other words, the average saprolite thickness at
496 a site may reflect large-scale controls like climate or tectonic stress, while smaller-scale
497 lateral heterogeneity must have local causes, like variations in fracture density or com-
498 position.

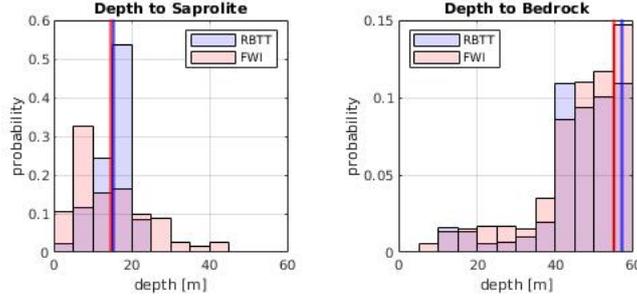


Figure 12. Overlain histograms of the depth to saprolite (left) and intact bedrock (right) in the FWI (red) and FATT (blue) models. The thick vertical lines indicate averages of the distributions displayed in the histograms.

499 Our results raise fundamental questions about the extent to which CZ architecture
 500 is controlled by large-scale forcing functions like climate, topography, and tectonic stress,
 501 versus local, smaller-scale characteristics of the bedrock. While past work has provided
 502 useful theories for the role of large-scale processes on CZ structure, our results suggest
 503 that smaller-scale factors also play an important role, as variability in bedrock charac-
 504 teristics over lateral scales of tens of meters imparts profound impacts on the overlying
 505 CZ architecture. We anticipate a concordance between the scale of forcing functions and
 506 their products. Seeking the signal of top-down processes like climate in CZ architecture
 507 will thus likely require comparing larger-scale averages across sites to filter out local vari-
 508 ability (e.g., Callahan et al., 2022). We expect that future applications of the FWI work-
 509 flow developed here will provide both new ideas and new hypothesis tests about the state
 510 and evolution of Earth’s critical zone.

511 6 Conclusions

512 In this study, we present an FWI workflow specifically tailored to study weather-
 513 ing patterns in the CZ. Using existing and accessible open source packages, we show how
 514 forward and adjoint modeling rooted in the spectral element method can be used to in-
 515 vert surface and body waves to constrain V_s and V_p . Our FWI results agree significantly
 516 better with borehole data than previously published FATT models. This, along with syn-
 517 thetic FWI experiments, bolsters confidence in our findings, which show remarkable het-
 518 erogeneity in the CZ, previously undetectable using traveltime tomography. We hypoth-

519 esize that local heterogeneity in Earth’s weathering engine reflects local variations in bedrock
520 composition and structure, including fracture density, foliation, and mineralogy. We sug-
521 gest that FWI can be used to investigate a wide range of important CZ processes at smaller
522 scales than previously possible.

523 **7 Open Research**

524 All seismic data and borehole logging data have been uploaded to a Zenodo repos-
525 itory (<https://doi.org/10.5281/zenodo.8219762>) and MATLAB codes for source estima-
526 tion as well as a copy of our fork of SeisFlows will be uploaded pending acceptance of
527 this.

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