Full model wavenumber inversion (FMWI): identifying sources of information for the elusive middle model wavenumbers

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Running head: **Middle model wavenumbers?**

ABSTRACT

We recognized over the years that our conventional surface seismic recording can effectively identify two main features of the Earth: its seismic propagation attributes and those attributes resulting in echoes or reflections. Thus, the resulting expression of the Earth is dominated by the generally smooth (long wavelength) features that control wave propagation, which we use to invert for the short wavelength features causing reflections in a process we refer to as migration velocity analysis (MVA) and imaging, respectively. The features of the Earth that fall in between these two model scales: the middle wavenumbers, have been elusive, which is a dilemma for full waveform inversion (FWI) as we need to build the full velocity model (a broad band of model wavenumbers). We analyse the middle model wavenumber gap, but focus more here on potential sources of information for

20 such middle model wavenumbers. Such sources include regularization, objective function
21 enhancements, and multi scattered energy. Regularization, provided by a total variation
22 constraint admits middle and high model wavenumbers components into the model to en-
23 force the model's compliance with such a constraint. As opposed to minimizing the total
24 variation, such a constraint merely reduces the model space, and thus, these injected middle
25 model wavenumbers are as good as the projected data information to the reduced model
26 space. Such data information includes large offsets, but also multi scattered energy, in
27 which the energy through wave path and scattering updates can admit more of the elusive
28 middle wavenumber information that comes from the data. The combination of the right
29 level of allowable model variations with the added data information from large offsets and
30 multi scattering can help in filling the elusive middle model wavenumber gap and admit
31 plausible models.

INTRODUCTION

32 The recorded pulses of seismic waves originating from an active source and penetrating the
33 Earth include generally information related to the average velocity of the propagating wave,
34 manifested in the traveltimes it took for the pulse to arrive, but more importantly, possibly
35 some information of where it bounced from, usually referred to as velocity contrasts (Aki and
36 Richards, 1980). The bounce location information (imaging) requires more than one pulse
37 measurement from the same bouncing interface, providing directional information (Yilmaz,
38 2001). The traveltimes and bounce roles were highlighted in Claerbout (1985), where he
39 attempts to describe the data sensitivity to the various velocity model scales.

40 The objective of a full waveform inversion (FWI) implementation is to predict the veloc-
41 ity information within a domain of interest that is missing from the initial (known) model
42 of the subsurface. The missing velocity information is iteratively added to the known model
43 until the resulting combined model is able to produce simulated data that resembles the
44 recorded data. In doing so, FWI uses the difference between the recorded data and the
45 simulated ones to update the velocity model by mapping this difference to updates in the
46 model space (Tarantola, 1984). These updates are extracted from wavefields, and thus,
47 they are sinusoidal in nature best expressed by wavenumber components in the space do-
48 main (Wu and Toksaz, 1987; Sirgue and Pratt, 2004; Alkhalifah, 2016a). So to predict the
49 missing velocity information required to produce the desired simulated data, we will need
50 FWI to find all the wavenumber components that could properly represent such missing
51 information. The initial model often contains only smooth components, low wavenumber
52 information. So FWI needs to inject wavenumbers into the model from low to high as we
53 have to satisfy the propagation accuracy requirement for various frequencies to avoid cycle

54 skipping (Bunks et al., 1995; Pratt et al., 1996; Alkhalifah, 2014).

55 The middle wavenumber gap is dependent on our recording geometry, velocity model,
56 and the recorded frequency band (Wu and Toksaz, 1987). For surface seismic data, the
57 gap often widens with depth due to the limited illumination angles. Deeper parts of the
58 model also suffer from natural physical limitations of wave propagation like energy loss
59 due to geometrical spreading and dispersion, which also attenuates the high frequency
60 content. The dilemma in resolving the deep model portion from surface seismic data is an
61 ongoing challenge. Attempts to fill the middle wavenumber gap sparked the push for more
62 low-frequency acquisition (Bunks et al., 1995; Pratt et al., 1996; Virieux and Operto, 2009)
63 and for acquiring larger offsets (Sirgue and Pratt, 2004), as well as, improving our ability to
64 estimate a good initial model for FWI (Xu et al., 2012; Ma et al., 2012; Fleury and Perrone,
65 2012; Wang et al., 2013; Alkhalifah and Wu, 2016b; Chavent and Plessix, 1999; Clement
66 et al., 2001).

67 In a previous paper, Alkhalifah (2016a) demonstrated the importance of accessing the
68 middle model wavenumbers and the necessity to build such model wavenumbers from low
69 to high. He emphasizes the case for using scattering-angle filtering to implement this
70 wavenumber continuation from low to high. However, the sources for accessing such miss-
71 ing middle model wavenumbers from the data were not addressed. In this paper, we will
72 investigate combining two, one of them often ignored, sources of middle wavenumber infor-
73 mation. We will show the potential of these sources of model wavenumber information, but
74 also outline their limitations. Most importantly, we seek to gain knowledge on how to use
75 such information in waveform inversion. We will start the paper by reviewing FWI from
76 the model wavenumber standpoint, and then shift to the issue of the middle wavenumber
77 gap. Finally, we investigate the role of regularization and multi scattering in providing

78 such middle model wavenumbers. We will support the theoretical assertions with numerical
 79 examples.

FULL WAVEFORM INVERSION IN A NUTSHELL

80 The difference between the recorded field data and data simulated in our computing devices,
 81 using the same experiment setup, and under our best assumptions of the physics of wave
 82 propagation inside the Earth, is used to update the Earth’s acoustic, elastic, and possibly
 83 anisotropic model of the Earth. This update is often implemented in an iterative framework
 84 we refer to as full waveform inversion (FWI). So we repeatedly map the data difference
 85 (between field and simulated data, we refer to as residual) to updates in the model using
 86 a linearized approximation of an otherwise nonlinear relation between model and data.
 87 If such difference between the field and simulated data decreases over iterations, we are
 88 converging. However, we often ask ourselves, what are we converging to? We often desire
 89 the minimum difference (global minimum) and here we will offer approaches to help do so.
 90 The global minimum ability to represent the true velocity model depends on the accuracy
 91 of our physical representation of the Earth (simulation) and our ability to illuminate the
 92 model space, or impose the proper constraints. The measure of difference can be performed
 93 in many ways, the most popular is given by a simple point-by-point subtraction adhering
 94 to the least square l_2 norm objective function first suggested within the framework of FWI
 95 by Tarantola (1984)

$$E_{FWI}(m) = \sum_i |d_{o_i} - d_{s_i}(m)|^2. \quad (1)$$

96 We define i as the source index, d_{o_i} as the observed data, $d_{s_i} = u_s(\mathbf{x}_{s_i}, t)$ as the modeled
 97 synthetic data measured at the surface, $z = 0$, and $m(\mathbf{x})$ as (any form of) the velocity

model described in space using the vector $\mathbf{x} = \{x, y, z\}$, along the Cartesian coordinates, with t as time. From this point on, and for simplicity, but without the loss of generality, we represent wavefields and data in the frequency domain. In this case, the modeled wavefield, u_s , satisfies the following wave equation:

$$L(m)u_{s_i} = f(\omega)\delta(\mathbf{x} - \mathbf{x}_{s_i}), \quad (2)$$

for a particular source location, $\mathbf{x}_{s_i}$, and f is the source function given in the frequency domain, with

$$L(m) = L^*(m) = \nabla^2 + \omega^2 m(\mathbf{x}), \quad (3)$$

for the case of an acoustic isotropic constant-density Earth, where ω is the angular frequency and ∇^2 is the Laplacian operator ($= \nabla \cdot \nabla$, where ∇ is the gradient). In this case, $m(\mathbf{x})$ is given by the slowness squared. However, the Helmholtz operator, L , can have differing forms to represent more complex physics, but for the purpose of focusing on model wavenumbers, we will stick with the simplest form, which happens to render the operator self adjoint. The gradient corresponding to such an objective function is given by (Tarantola, 1984)

$$R_{FWI}(\mathbf{x}) = \Re\left\{\frac{\partial L}{\partial m} \sum_i u_{s_i}(\mathbf{x}) L^{-1} \sum_j \delta(\mathbf{x} - \mathbf{x}_{r_{ij}})(d_{o_{ij}} - d_{s_{ij}})^*\right\}, \quad (4)$$

where $\mathbf{x}_{r_{ij}}$ are the locations of the receivers for source i , and j is the receiver index. The gradient (as a vector) points to the objective functional steepest descent direction in the model space. An often used simple update of the model, is to combine this steepest descent vector with a line search for a minimum.

Such Born approximation based gradients, which correspond to the interaction of a

115 source wavefield with the adjoint residual wavefield, are space domain functions with a har-
 116 monic nature courtesy of the wavefields used in computing them. These harmonic features,
 117 using a local plane wave decomposition of the wavefields, can be expressed as a function
 118 of a model amplitude (radiation pattern), and a model wavenumber vector. The model
 119 wavenumber vector describes the resolution and dip of a potential gradient point (esti-
 120 mated model perturbation). Based on diffraction tomography, and assuming locally plane
 121 wavefields for the state and adjoint state wavefields, the model wavenumber vector, $\mathbf{k}_m$, is
 122 given by (Miller et al., 1987; Jin et al., 1992; Thierry et al., 1999),

$$\mathbf{k}_m = \mathbf{k}_s + \mathbf{k}_r = 2\frac{\omega}{v} \cos \frac{\theta}{2} \mathbf{n}, \quad (5)$$

123 which depends on, among other things, the angular frequency, ω , with a direction guided by
 124 a unit vector, $\mathbf{n}$, normal to a potential scattering interface. Here, $\mathbf{k}_s$ and $\mathbf{k}_r$ are the source
 125 and receiver (or any state and adjoint state) wavefield wavenumber vectors, respectively, at
 126 the model point, with θ as the angle between these vectors (the scattering angle), and v
 127 ($= \frac{1}{\sqrt{m}}$) is the velocity at the model point. For multi scattered energy, the state and adjoint
 128 state could include perturbed wavefields. Nevertheless, equation 5 still applies under the
 129 local plane wave approximation.

THE MIDDLE WAVENUMBER GAP

130 The updates we expect from FWI consists of, as Mora (1988) so eloquently described, trans-
 131 mission and scattering parts. The transmission part is provided by equation 4 when the
 132 scattering angle between the state and adjoint state wavefields is around 180° . It is depen-
 133 dent on the dominant wavelength along the wavepath, and provided by the first Fresnel zone

134 (Williamson, 1991). Such updates, according to diffraction tomography (equation 5) provide
 135 low wavenumber (long wavelength) wavepath updates. For deeper targets, such transmission
 136 updates are also provided by wavepath updates along reflection paths. For transmissions
 137 in all cases, equation 5 is combined with the first fresnel zone limit (Williamson, 1991) to
 138 provide the resolution range for transmissions, and that range starts at zero along the ray
 139 path. The upper bound for transmissions can be extracted, for a homogeneous background,
 140 from simple trigonometric relations, and thus, is given by (Alkhalifah, 2016b):

$$k_{max} = 2k \frac{\sqrt{1 + 4lk}}{1 + 2lk}, \quad (6)$$

141 where $k = \frac{\omega}{v}$, l is the length of the wavepath, for example from the source to the receiver.
 142 Note that for zero offset ($l = 0$), equation (6) provides the same resolution as equation (5)
 143 for $\theta = 0$. For large l , $k_{max} \approx 2\sqrt{\frac{k}{l}}$, which implies, as expected, resolution is inversely
 144 proportional to wavepath length for transmissions. In a homogeneous background, formula 6
 145 applies to reflections from plane interfaces, where the l corresponds to the path from the
 146 source to the reflector and back to the receiver. If the energy corresponds to scattering from
 147 a point scatterer, then l corresponds to the wavepath from the point scatterer (secondary
 148 source) to the source or receiver. This path from a scatterer is far shorter, and thus,
 149 according to equation 6, provides higher resolution. This phenomenon will be described
 150 later in multi scattering.

151 So the model wavenumbers we may expect at a point in the subsurface from far field
 152 transmission data (i.e. diving waves or reflection wave paths) range from zero to $2\sqrt{\frac{k}{l}}$.
 153 For reflections, the corresponding model wavenumbers range from $2k \cos \frac{\theta_{max}}{2}$ to $2k$, where
 154 θ_{max} is the maximum scattering angle, and for conventional reflection data it is tied to

155 the maximum offset. So the inherent gap in the model wavenumber build up from surface
156 seismic data is approximately proportional to $\cos \frac{\theta_{max}}{2} - \sqrt{\frac{1}{kl}}$, granted this quantity is
157 positive. So for deeper model points where the reflection wavepath can be an order longer
158 than the wavelength, and the maximum scattering angle is usually small for conventional
159 surface seismic acquisition, the gap could be wide.

160 In light of Gerhard Pratt’s diagram that outlines the wavenumbers recovered from the
161 discrete frequencies used in a frequency continuation strategy (Sirgue and Pratt, 2004), we
162 show in Figure 1 such a diagram in which we include the wavenumbers extracted usually
163 from imaging and tomographic methods. So the wavenumbers recovered (given in yellow)
164 from reflections in FWI is governed by equation 5, which constitutes the higher wavenum-
165 bers. While diving waves and tomographic methods based on reflections provide lower
166 wavenumbers. At depth, the maximum offset-to-depth ratio controlling the lower bound of
167 the higher wavenumbers reduces, and the length of the wavepath, whether it corresponds
168 to reflections or diving waves, increases causing the upper bound of the lower wavenumbers
169 to decrease and the middle wavenumber gap to increase. In Figure 1, we also suggest that
170 regularization and multi-scattered update energy can fill some of the gap. In fact, lim-
171 ited to conventional sources of information, and no constraints on the model, such middle
172 wavenumbers are unattainable and in the next section we try to show what that means.
173 As illustrated in Figure 1, the middle model wavenumbers do not have a fixed range; they
174 depend on the data and the background model, but for the purpose of this study, the middle
175 model wavenumbers correspond, by this definition, to the gap we face in conventional FWI.

Simple model test

We consider a one-dimensional model made up of three layers, or more importantly two interfaces, in a 2D experiment. Figure 2a depicts the one dimensional depth model in blue. The peak frequency of the source wavelet is 30 Hz, with a spectrum of frequencies ranging between 3 Hz and 80 Hz, a typical band for real seismic recorded data nowadays. The source spectrum mapped to wavenumber using the velocity of the first layer is shown in Figure 2b in green. The initial model, which is kinematically accurate, but smooth is shown as the black curve in Figure 2a. Figure 3 shows a part of the shot gather corresponding to the true model (left side) and part of the gather corresponding to the initial model on the (right side). Considering the 1D nature of the model, both gathers are symmetric with respect to zero offset. The direct arrivals and mainly two reflections are apparent. We use an absorbing boundary condition on all surfaces. The multiple reflection between the two layers, in which the apex should appear at 2 s time, is weak. For the initial velocity model, in which the reflectors are smoothed, the reflection energy, as expected, increases with offset. Such reflection energy is kinematically accurate supporting the kinematic accuracy of the initial velocity model. Thus, this velocity model should place all wavenumbers approximately in its accurate position, mitigating the FWI nonlinearity (we are within the basin of attraction of the global minima). Since we are dealing with a 1D model and noise free data, we simulate the predicted data and calculate the gradient for a single shot, and then stack the gradient laterally to get the effect of full fold coverage of the displayed profiles. Our objective here and throughout the paper is to identify what it takes to recover the difference between the initial and true model in this simple but representative experiment. Though the Earth is often more complex, we seek to analyze the inverted models in terms of wavenumber retrieval capability. For the various tests using this model, we will stop at 15 iterations of the basic

200 steepest descent with Golden-section line search updates (Press et al., 1986). Though for
 201 certain approaches, like including multi scattering, the iteration might be more expensive,
 202 the purpose here is to evaluate what are we getting in terms of model wavenumbers from the
 203 various considerations. The objective function considered in this paper is the least square
 204 misfit shown in equation 1.

205 Using the classic single scattering FWI, Figure 2a shows the inverted model in red for
 206 a maximum offset of 1000 m after 15 iterations. The resulting model suffers mainly from
 207 the elusive missing middle model wavenumbers as well as missing some high wavenumbers
 208 beyond the frequency band (thus, Gibb’s phenomena). This fact is reflected in Figure 2b,
 209 which shows the spectrum of the model difference between the initial and the true model
 210 (i.e., true perturbation) plotted in blue, together with the spectrum of the inverted dif-
 211 ference (i.e., inverted perturbations) plotted in red. On the same Figure, the black curve
 212 corresponds to the model wavenumbers provided by the initial model, which are low. The
 213 green curve, which corresponds to the spectrum of the source wavelet mapped to wavenum-
 214 bers, and is the same for all experiments, acts like a filter applied to the inverted model;
 215 as a result, a poor fit of the inverted model at the high end. The mismatch between the
 216 true difference and the inverted one also happens at the low end (defined here and through-
 217 out as the middle wavenumbers, which is the region between 0.02 and 0.1 of normalized
 218 model wavenumbers, see Figure 2b). As mentioned earlier, this range for the middle model
 219 wavenumber was chosen because it represents the largest misfit between the true perturba-
 220 tion and the inverted one using conventional FWI, or in other words, the gap.

221 For a larger maximum offset of 3000 m (shown in Figure 2c), we seem to match the
 222 middle wavenumbers better (see Figure 2d), but at the expense of the high wavenumbers.
 223 The middle wavenumber improvement is expected as the scattering angle increases with

offset, thus, adding more lower wavenumbers. Therefore, resolution is expected to decrease, as we try to match the imperfect inverted model to larger offsets (more iterations are possibly required for more data). This behavior has an equivalency in imaging as resolution of the image decreases as we add information from larger offsets (the stretching phenomena). However, in imaging, the larger offsets are needed to enhance the signal to noise ratio. In FWI, and as an iterative process, we can control what data to include. Thus, we probably can focus the inversion on the near offsets at later iterations. This possibility is given by the fact that FWI is an iterative process and we end up adding or subtracting wavenumbers per iteration. By focusing on the short offsets at the end, we can inject higher resolution information (i.e., shorter wavelengths).

SOURCES FOR MIDDLE WAVENUMBER INFORMATION

We will look into two potential sources of middle wavenumber information at depth. One is based on assumptions we make on the model by imposing constraints on it. So middle and high wavenumbers are injected into the model by an assumption made of the model. The other is based on utilizing parts of the data, namely multi scattering, not often utilized in the update procedure. We promote such utilization in wavepath and scattering updates. An essential part of making this multi scattered energy contribute accurately is the optimization nature of its contribution. Meaning, we ensure that such updates through Born modeling fits the residuals in the data corresponding to multi scattered energy (Alkhalifah and Wu, 2016a).

243 Regularization

244 The options for regularization are many and they usually try to conform the model to some
 245 form we expect it to comply with. In such conformation, regularization is expected to alter
 246 the wavenumber content and, in some cases, to inject middle wavenumber information.
 247 In fact, any constraints, for example, that promote reduced variation in the model will
 248 explicitly reduce the sinusoidal nature of the model. This will inherently inject model
 249 wavenumbers that are not present in the band limited nature of our wavefield to force a
 250 more white spectrum. There are a slew of methods that aim to reduce the variation in the
 251 model and enhance blockiness (Portniaguine and Zhdanov, 1999; Guitton, 2012), like the
 252 minimum gradient support (MGS) and many others. One very popular constraint, often
 253 applied on the model to capture sharp interfaces, is limiting the total variation (TV) in the
 254 model. We will focus on the TV regularization, as opposed to the other methods, as it is
 255 widely used. However, many of the conclusions we will arrive to logically applies to the
 256 other methods. TV is a measure of the variation using the following formula:

$$J_{TV}(m) = |\sqrt{\nabla m \cdot \nabla m + \epsilon}|_p, \quad (7)$$

257 where p defines the norm, which is one for total variation ($p = 1$), implying a simple sum-
 258 mation over space coordinates, and ϵ is a small positive number to mitigate the singularity
 259 at zero. The operator ∇ , as mentioned previously, stands for the gradient. If we set $p = 2$
 260 and $\epsilon = 0$, we obtain the classic Tikhnov regularization. Here, however, we focus on the TV
 261 regularization as an example. For wavefields, total variation acts as a harmonic normalizer.
 262 In other words, it tries to reduce the sinusoidal nature of the model, which induce large
 263 variations.

264 The TV ($p = 1$) gradient is given by

$$\nabla_m J_{TV} = \nabla \cdot \frac{\nabla m(\mathbf{x})}{\sqrt{\nabla m \cdot \nabla m + \epsilon}} = \frac{\nabla^2 m(\mathbf{x})}{\sqrt{\nabla m \cdot \nabla m + \epsilon}} - \frac{(\nabla m \cdot \nabla m) \nabla^2 m(\mathbf{x})}{\sqrt{\nabla m \cdot \nabla m + \epsilon}^3} \quad (8)$$

265 Since for $\epsilon = 0$, the gradient equals zero as the two terms become identical, the gradient
 266 is given mainly by the Laplacian of the velocity model. This operator increases the energy
 267 of the higher wavenumber components, divided by the local variation. The role of the
 268 denominator in the gradient in equation 8, which is the local variation (amplitude of change)
 269 depends on the size of ϵ . However, this local variation is key in introducing additional
 270 middle- and high-model wavenumber information. To understand its role, let consider a
 271 one dimensional velocity model with two wavenumber sinusoidals, a low wavenumber (long
 272 wavelength) component inherent in the model courtesy of the initial guess ($k_1 \approx 0$), and a
 273 high wavenumber (short wavelength) component introduced by the inversion gradient of a
 274 missing reflectivity ($k_2 \gg 0$). So the velocity model is given by

$$m(z) = m_0 + A_1 \sin k_1 z + A_2 \sin k_2 z, \quad (9)$$

275 and the gradient of the total variation:

$$\nabla_m J_{TV} = - \frac{\epsilon(A_1 k_1^2 \sin k_1 z + A_2 k_2^2 \sin k_2 z)}{(A_1^2 k_1^2 \cos^2 k_1 z + A_2^2 k_2^2 \cos^2 k_2 z + A_1 A_2 k_1 k_2 (\cos(k_1 + k_2)z + \cos(k_1 - k_2)z) + \epsilon)^{\frac{3}{2}}}. \quad (10)$$

276 From the above, the key element that has changed in the sinusoidal nature of the model is the
 277 addition of the wavenumbers $k_1 + k_2$ and $k_1 - k_2$. The first introduces high wavenumbers,
 278 while the latter introduces middle wavenumbers to the model when the difference between
 279 k_1 and k_2 is large. The amount of wavenumber introduction decreases with an increase in

280 ϵ .

281 The total variation can be included in the objective function, as we try to minimize
282 it, as depicted by equation 8. We can also apply it as a constraint; that is we limit the
283 variation in the model to some predetermined value. We will utilize this approach in the
284 examples in this paper following the algorithm suggested by Zhu and Chan (2008). If we
285 apply it as a constraint, we limit the model space to those models that comply with the
286 constraint. There are many algorithms that can guarantee this compliance. Among those
287 are algorithms that project the update to a model space that complies with a constraint
288 like the projection onto a convex set (POCS, (Baumstein, 2013)).

289 We repeat the earlier (3-layers) numerical experiment, but with a total variation con-
290 straint. So we are seeking a model that fits the data and has a limited total variation.
291 The limit on TV is extracted from the total variation of the true model, which is in this
292 example equal to the TV of the initial model. The inverted model for the 1000 m offset
293 case after 15 iterations is shown in Figure 4a in red, and has a blocky shape similar to the
294 true model courtesy of the limited variation constraint. As a result, the spectrum of the in-
295 verted perturbation, shown in Figure 4b in red, seemingly predicted the high wavenumbers
296 slightly better, but failed to predict the middle wavenumbers well. As we use larger offsets
297 in the inversion, specifically up to 3000 m, we seemingly get a better fit between the true
298 (blue) and inverted (red) curves, as shown on Figure 4c. The model perturbation spectrum
299 shown in Figure 4d supports such an assertion, especially in correctly predicting the middle
300 wavenumbers. There are still some difference so let us examine what happens if we include
301 multi scattered energy in the update of FWI.

302 Multi scattering

303 Multi scattered energy is often ignored within the context of the FWI update. Though
304 inverted models may produce energy upon simulation that fits the multi scattered energy,
305 the update process, which is crucial for proper convergence, often does not utilize such
306 energy. The critical role of multi scattering as it pertains to our objective is the additional
307 model wavenumbers it may admit. Specifically, the additional scattering will eventually
308 offer additional information in its unique wavepath, and often scatter at additional angles.
309 In fact, if the additional scattering is caused by an object acting as a point scatterer (smaller
310 than a fourth of the dominant wavelength), the scattering will enhance the resolution of
311 wavepath updates, especially if the path between the scattering object and the sensor is
312 short. Figure 5a displays an example where such a phenomenon may occur, and that is the
313 complex top of a salt body. In this part of the Sigsbee model, many areas of the top of
314 the salt body may result in scattering of certain wavelengths resulting in short wavepath
315 updates in FWI between scattering points (Figure 5b). So the wavepaths for the Sigsbee
316 model though corresponding to zero offset, which often provides limited information for
317 inversion, with double scattering it resulted in additional scattering angles (Figure 5a) and
318 additional wavepath updates of a shorter nature. The top of the salt is a strong scatterer of
319 energy, and thus, we may expect that such energy will be recorded. The enhanced nonlinear
320 model update for FWI promises to offer more information, including middle wavenumbers.

321 We again use our 3-layer one-dimensional model in a two dimensional inversion setup
322 using this time multi-scattered energy. Like before, we perform 15 steepest descent with
323 line search iterations, but now including energy corresponding to fourth-order scattering
324 (Alkhalifah and Wu, 2016a). For the 1000 m maximum offset case, shown in Figure 6a,

the inverted model in blue suffers much of the limitations of the single scattering case. The updates here are pure perturbation updates. No background wavepath updates were included as the initial model here represents the background accurately. So the difference between the spectrum of the inverted model perturbations in blue in Figure 6b and the true one in red is large at the high and low ends. Having a larger maximum offset given by 3000 m in Figure 6c produced an inverted model given in blue that is closer to the true model given in red. The model perturbation spectrum shown in Figure 6d supports such an assertion as the middle model wavenumbers of the inverted perturbation in blue better fits the true perturbation in red. The lack of higher wavenumbers in the inverted perturbations is the result of using larger offsets as we saw earlier in the single scattering case (Figure 2d).

Compared to the single-scattering update result, we have improvements with multi scattering updates overall (or in average). However, the results of the multi scattering update are more sinusoidal, due to the admission of more higher wavenumbers over a narrow band, and this is true more for the shorter offset case. Thanks to the additional high wavenumbers, the multi scattering update results capture the sharpness of the interface better than the single scattering update result. It is important to reiterate that the multi scattering updates are not optimized, which means it is prone to the divergence of the scattering series. In the Marmousi example we will see later, we optimize the updates (fit it to the residuals, like least-squares migration). It, also, implies that the multi-scattering update results include more (possibly unwanted) variations, and thus, it is in more need for a constraint to reduce the variations.

If we add a total variation constraint to the mix, we should expect a more blocky solution, as the variations due to the sinusoidal nature of wavefields are mitigated. Figure 7a shows the inverted model in blue for the case of a 1000 m offset after 15 iterations. It seems to

349 be similar to the single scattering result, but with slightly higher accuracy in some regions,
 350 like the velocity of the second layer up shallow. The model spectrum, shown in Figure 7b,
 351 confirms the higher agreement of the inverted perturbation in blue to the true perturbation
 352 in red. If we use offsets up to 3000 m, the inverted model in blue in Figure 7c agrees well
 353 with the true model in red. This is further supported by the agreement in the spectrum
 354 shown in Figure 7d. So the additional data from the larger offsets and additional scattering
 355 managed to inject enough information into the model as it adheres to the TV constraint.
 356 The next question is how well and fast we managed to fit the data.

357 **Data fitting**

358 A crucial component of the experiments above is the convergence speed in which we managed
 359 to fit the data (an important goal considering we collected such data). We have restricted all
 360 the tests to fifteen iterations to allow for a fair comparison. The shot gather data residuals
 361 between the true and initial model is shown in on the left side of Figure 8. It represents
 362 the starting point of the misfit, which, as expected, reflects the need to predict model
 363 components that will reduce such reflection residuals. The data misfit for each maximum
 364 offset test (1000 m and 3000 m) is the same at the first iteration as we start from the same
 365 initial model so we normalize each offset experiment by the misfit at the first iteration, shown
 366 in Figure 8. Figure 9a shows the misfit based on the l_2 norm objective function, normalized
 367 by its value at the first iteration, as a function of iteration for the case of a maximum
 368 offset of 1000 m for the four experiments: conventional single scattering update in solid red,
 369 including fourth order scattering in the update in solid blue, and adding the TV constraint
 370 to both cases are the dashed counterparts. For the short offset case, and with limited middle
 371 model wavenumber information, the TV led to good fitting early, but ultimately, the low

372 and middle wavenumbers were guided by the quest to reduce the variation (less constraints
 373 from the data), and the fit was worse in both the single and the multi scattered update
 374 cases. The data residuals at the last iteration for the 1000 m offset inversion for the four
 375 cases are shown in Figures 10a, 10b, 10c, and 10d, respectively. In all cases, the residuals
 376 are mainly reduced at the near offset as the inversion is focussed on fitting 1000 m offset.
 377 However, the level of misfit at the far offset is larger in the case of using the TV constraints.
 378 On the other hand, the TV constraints admitted lower misfits at the near offset, where the
 379 data misfit is contributing to the update.

380 For the 3000 m offset case, as shown in Figure 9b, the total variation constraint helped
 381 the data fitting. In fact, for the multi scattering update case and after 8 iterations, the
 382 convergence was fast. So the constraint, if accurate, acts as a bound helping to reduce
 383 the model space to those that comply with the constraint. The constraint also acts as
 384 an interpolant of wavenumbers, but like any interpolation operator, it is as good as the
 385 information we interpolate from. With multi scattering in the FWI update and large offsets,
 386 we interpolate from rich sources of data information. The data residuals at the last iteration
 387 for the 3000 m offset inversion for the four cases are shown in Figures 11a, 11b, 11c, and 11d,
 388 respectively, after multiplying them by a factor of 20 (left flanks of the shot gathers). The
 389 scaling of the residuals was needed to make them observable for this 3000 m offset case,
 390 compared to the 1000 m offset, which was shown at the same scale as the shot gather.
 391 Otherwise, for the 3000 m offset models, the residuals plotted at the same scale would have
 392 shown near zero values everywhere. So as expected, with the 3000m offset inversion we
 393 obtain better fit to the data at far offsets. We also obtain the best fit (least residuals) for
 394 the case of using multi scattering updates and a TV constraint as shown in Figure 11d.

A MARMOUSI TEST

We next test the benefits of including multi-scattering updates and the TV constraint on the Marmousi model dataset. Figure 12a shows the Marmousi model (Versteeg, 1994). We use only 3 Hz frequency data in this test for simplicity and since our objective is to highlight the advantages of including multi-scattering updates and the TV regularization. We use a free surface boundary condition on the top boundary. Such data were acquired assuming every point on the surface at a 25 m spacing as a receiver. Sources are placed at a 100 m spacing. We start with a smoothed version of the Marmousi shown on Figure 12b, as the initial model. Figure 13a shows the inversion result after 20 iterations of optimized (where the update fits the residual, Gauss Newton) single scattering updates. The inverted model, considering we use only 3 Hz frequency data, has some of the expected features of the true model, but also is relatively jittery (no smoothing was used here). With the same number of iterations of double scattering optimized updates, the inverted model shown in Figure 13b shows generally more of the true velocity details than its single scattering counterpart, and less harmonics as more model wavenumbers are included. Since we use the direct solver to evaluate the Helmholtz operator, the cost of using double scattering in the updates of FWI is only fractionally higher than using only single scattering. The full Hessian includes double scattering, however, not the properly weighted kind (Alkhalifah and Wu, 2016a). In other words, it does not utilize the Gauss-Newton Hessian of the second-order scattering term. Such a Gauss-Newton weighting function can be extracted mathematically from the third-order term of the generalized Taylor series expansion of the objective function with respect to the model, which we practically ignore.

When we include total variation minimization in the objective function, we expect the

417 result to be more blocky. Contrary to using TV as a constraint, the minimization approach
 418 spares us the need to define the constraint value, which might be hard in complex models
 419 with low velocity zones. Figure 14a shows the inverted model for the 3Hz data with mini-
 420 mizing the total variation and after 20 iterations of single scattering optimized updates. The
 421 model has a more blocky look to it. If we utilize double scattering in the update, as shown
 422 in Figure 14b, the inverted model appears to be cleaner than its single scattering counter-
 423 parts (less jitters), which is courtesy of the additional model wavenumbers constrained by
 424 including double scattered energy.

DISCUSSION

425 The role of total variation (TV) as a constraint is interesting. In the 3-layer numerical
 426 examples, we use the true model total variation as a constraint. In practice, we can rely on
 427 the initial model for that information. Actually, the initial model in the numerical examples
 428 has the same TV as the true model. So as we constrain the total variation, the data become
 429 crucial in figuring out the accurate velocity information within such a constraint. In fact, for
 430 the low-to-middle wavenumber end of the spectrum of the model, we are more prone to errors
 431 if data are not capable of guiding the velocity within the constrained model space. So with
 432 the larger offsets, more data, we noticed that the TV constraint helped the convergence. In
 433 this case, the TV acts in interpolating the data fit into the missing model wavenumbers. On
 434 the other hand, with only short offsets, the TV constraint slightly harmed the convergence.
 435 In deciding the TV constraint, we will have to be careful when we have, or expect, low
 436 velocity zones. If velocity is only increasing or decreasing with depth, the total variation
 437 is given by the maximum and minimum velocity. In many cases, we will need to relax the
 438 constraint to allow for low velocity zones to develop. This procedure can be done at later

439 stages in the iterative process of FWI as well.

440 Likewise, multi scattering also provides more model wavenumber information extracted
441 from the measured data. Of course, this conclusion corresponds to updates in the pertur-
442 bations. Updates in the wavepath of multi scattered energy should help the model building
443 problem even more so for large offsets. Combining TV with multi scattering updates pro-
444 vides the opportunity to use a lot of the data to find the optimal model in the constrained
445 space. The order of scattering needed depends on the strength of the multi scattered energy.
446 In the Marmousi example we only used double scattering and the improvements were clear.
447 If we expect in a region that interbed multiples are present, third order scattering might be
448 useful.

449 In the examples we shared, the power of TV (or possibly other) regularizations in admit-
450 ting middle model wavenumbers were clear. It seems to exceed those of the multi scattering
451 updates, as mutli scattering depends on the data and the strength of such energy in the
452 recorded data. Optimizing such multi scattering updates to fit the residuals helps en-
453 hance its role. Yet, the role of multi scattering based updates in introducing middle model
454 wavenumbers seems to be less than that admitted through regularization. However, we have
455 to remember that regularizations are assumptions we make on the model, and the resulting
456 model adhering to such assumptions (including the introduced middle model wavenumbers)
457 is as good as our regularization assumption.

458 The role of including multi scattering components in the FWI update process, as men-
459 tioned earlier, can potentially inject information at both the low and high end of the model
460 spectrum. Though multi scattering is synonymous with multiples and multiple reflections,
461 in FWI updates, our goal is not the treatment of multiples. Eventually, in all FWI, we

462 thrive to build a model that reproduces all the multiples in the data. If multiples exist, the
 463 nonlinearity of the FWI optimization problem is more severe. So nonlinear multi-scattering
 464 updates can help in the convergence regardless of the background velocity, as it is a higher-
 465 order approximation of the sensitivity of the data to the model. Even though the scattering
 466 series is not necessarily a convergent series, our implementation based on optimizing the
 467 updates does not suffer from such a problem (Alkhalifah and Wu, 2016a). In other words,
 468 the series is normalized to fit the data. In the examples in this paper, the scattering order
 469 was picked haphazardly. The purpose here is mainly to emphasize the role of higher-order
 470 scattering regardless of the order.

CONCLUSIONS

471 In this study, we highlighted potential sources for the elusive middle model wavenumbers
 472 needed to build more of the velocity model, which is also instrumental in helping our iterative
 473 inversion methods to converge. Regularization imposes certain assumptions on the model,
 474 and in our case we tested the minimizing or constraining of the total variation (TV) of the
 475 model. As a result, the TV injected some of the necessary model wavenumbers needed to
 476 adhere to the TV assumptions. The gradient of the total variation regularization reflects
 477 the wavenumbers that will be added to the model, and those often includes middle, as well
 478 as high, wavenumbers. However, those model wavenumbers are as good as data guides
 479 them. So additional data like large offsets and multi scattered energy in the update can
 480 help the constrained FWI converge *better* to a *better* model. A single frequency experiment
 481 on the Marmousi model demonstrated how we managed to expand the wavenumber band
 482 using multi scattered energy in the FWI update and total variation regularization.

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Figure 1: A schematic diagram showing the potential recovered model wavenumbers at a point in the model space as a function of frequency in the data (in this case, the offset-to-depth ratio seems to be small resulting in a large middle wavenumber gap). The addition of multi scattered energy with a total variation constraint has the potential to expand the yellow region of expected model wavenumbers.

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Figure 2: The inverted velocity using conventional FWI and its spectrum as a function of normalized vertical wavenumbers for a maximum offset of 1000m (a, b), and 3000m (c, d). Improvements due to larger offsets appear at the bottom of the first and second layers and in the third layer. In the wavenumber spectrum, we obtain a better fit in the low end of the spectrum for larger offsets, but deteriorating results at the high end.

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