High-resolution velocity estimation from surface-based common-offset GPR reflection data

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8 Summary

Surface-based common-offset ground-penetrating radar (GPR) reflection profiling is a popular 9 geophysical exploration technique for obtaining high-resolution images of the shallow 10 subsurface in a cost-effective manner. One drawback of this technique is that, without 11 complementary borehole information in form of dielectric permittivity and/or porosity logs 12 along the profile, it is currently not possible to obtain reliable estimates of the high-frequency 13 electromagnetic velocity distribution of the probed subsurface region. This is problematic 14 because adequate knowledge of the velocity is needed for accurate imaging and depth 15 conversion of the data, as well as for quantifying the distribution of soil water content. To 16 overcome this issue, we have developed a novel methodology for estimating the detailed 17 subsurface velocity structure from common-offset GPR reflection measurements, which does 18 not require additional conditioning information. The proposed approach combines two key 19 components: Diffraction analysis is used to infer the smooth, large-scale component of the 20 velocity distribution, whereas the superimposed small-scale fluctuations are inferred via 21 inversion of the reflected wavefield. We test and validate our method on two synthetic datasets 22

23	having increasing degrees of complexity and realism before applying it to a field example from
24	the Boise Hydrogeophysical Research Site (BHRS), where independent control data in the
25	form of neutron-neutron porosity logs are available for validation. The results obtained
26	demonstrate the viability and robustness of the proposed approach. Further, due to its efficiency,
27	both in terms of field effort and computational cost, the method can be readily extended to 3D,
28	which further enhances its attractiveness compared to multi-offset-based GPR velocity
29	estimation techniques.
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31	Abbreviated title: Velocity estimation from common-offset GPR data
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33	Keywords: Electrical properties; Hydrogeophysics; Electromagnetic theory; Ground
34	penetrating radar; Inverse theory; Wave scattering and diffraction.
35	
36	1 Introduction
37	Ground-penetrating radar (GPR) is a high-resolution geophysical exploration technique that

has the potential of providing images of shallow subsurface structure with a resolution in the meter to decimeter range (e.g., Knight 2001; Annan 2005; Klotzsche et al. 2018; Lai et al., 2018). Whereas borehole-based GPR transmission techniques have proven to be well-suited to full-waveform inversion approaches (e.g., Ernst et al. 2007; Klotzsche et al. 2019), estimating the detailed velocity structure of the subsurface from surface-based GPR reflection data is notoriously difficult. This is problematic because: (i) the overwhelming majority of GPR data are acquired in reflection mode along the Earth's surface; (ii) accurate velocity information is necessary for proper imaging of reflection data; and (iii) the high-frequency electromagnetic
wave velocity in the GPR regime has a strong and direct sensitivity to soil water content, which
is a key parameter for many hydrogeological, agricultural, and engineering applications (e.g.,
Huisman et al. 2003).

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One common approach for subsurface velocity estimation from reflection GPR measurements 50 is to collect data at multiple transmitter-receiver offsets and to perform either normal-moveout 51 (NMO) velocity analysis (e.g., Greaves et al. 1996; Huisman et al. 2003; Perroud & Tygel 2005) 52 or reflection tomography (e.g., Bradford 2008). With regard to NMO, the inherent assumption 53 of 1D horizontal layering means that it cannot effectively deal with the highly heterogeneous 54 velocity structures that are rather common in near-surface investigations. Although reflection 55 tomography is able to overcome this issue, it comes at a rather high computational cost and 56 requires inherently subjective horizon picking. Further, as pointed out by Bradford et al. (2009), 57 reflection tomography only recovers the large-scale component of the subsurface velocity 58 distribution that is needed to properly focus and image the GPR data, which is of substantially 59 lower resolution than the reflection image itself. The latter problem can be potentially 60 alleviated through waveform inversion approaches (e.g., Busch et al. 2012; Lavoué et al. 2014); 61 however their success so far has been limited due to the rather narrow range of reflection angles 62 and antenna radiation patterns that are highly complex, largely unknown, and site-dependent 63 (e.g., Lampe & Holliger 2003). Finally, a clear drawback of multi-offset GPR acquisitions is 64 their high cost in terms of acquisition time, which increases approximately linearly with the 65 considered number of transmitter-receiver offsets for the common case of GPR systems having 66

a single transmitter and receiver antenna. Indeed, such surveys become largely impractical in
the context of long 2D profiles and, particularly, 3D acquisitions.

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For the above reasons, the vast majority of surface-based GPR reflection surveys are performed 70 using the traditional bi-static, common-offset approach, where a single transmitter-receiver 71 antenna pair, separated by a small fixed distance, is incrementally moved along the 72 measurement profile (e.g., Annan 2005). While the estimation of the subsurface velocity 73 distribution from such data is substantially more difficult than for multi-offset GPR surveys, 74 significant efforts have been made during the past decade because of the high potential rewards. 75 In this regard, Schmelzbach et al. (2012) present an impedance inversion approach for 76 common-offset GPR data that is based on a convolution model for the GPR traces, where 77 borehole dielectric permittivity or porosity logs are used to recover the low-frequency part of 78 the velocity structure that cannot be obtained from the reflection data. Zeng et al. (2015) and 79 Liu et al. (2018) adopt similar approaches to estimate the distribution of soil water content and 80 to characterize buried archaeological remains, respectively. Xu et al. (2021) also assume a 81 convolution model for the GPR traces, but combine stochastic simulation with simulated 82 annealing optimization in order to generate velocity realizations that honor the GPR 83 measurements and borehole porosity log data along the profile. Forte et al. (2013; 2014) assume 84 a locally 1D layered subsurface structure and use picked reflection amplitudes to recursively 85 estimate the GPR velocity in a series of identified subsurface layers, in which the velocity is 86 assumed constant. Other authors estimate the spatial distribution of GPR velocity from 87 common-offset data via the analysis of diffractions present in the recordings. Novais et al. 88

(2008) use velocity continuation to generate several migrated sections and analyze the 89 associated diffraction focusing to build a root-mean-square (RMS) velocity model. Clair & 90 Holbrook (2017) apply the seismic diffraction imaging and velocity analysis workflow 91 proposed by Fomel et al. (2007) to common-offset GPR data in order to estimate snow water 92 equivalent. Yuan et al. (2019) employ a similar approach to characterize the velocity structure 93 of surficial chalk deposits. Although all of the above methods have the ability to estimate 94 subsurface properties from common-offset GPR measurements, they all suffer from inherent 95 limitations. Notably, the reflection-based methods have the potential to provide high-resolution 96 results, but they generally require complementary information such as borehole logs, which are 97 usually not available. Conversely, diffraction-based methods require a suitably dense and even 98 distribution of diffractions in the data and, even under ideal circumstances, can only resolve 99 the large-scale velocity structure. 100

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In this study, we present a novel velocity estimation method for surface-based common-offset 102 GPR reflection data that combines the advantages of the reflection- and diffraction-based 103 techniques described above. To estimate the low-frequency background velocity field, 104 diffractions are separated from the unmigrated GPR data and subjected to migration velocity 105 analysis based on a prescribed focusing measure. After migrating the GPR data using the 106 derived velocity field, the reflected wavefield is isolated and used to deduce the small-scale 107 velocity fluctuations. The latter is accomplished via sparse inversion based on an iteratively 108 reweighted least-squares strategy assuming a convolutional model for each GPR trace. The 109 final high-resolution velocity distribution is obtained by combining the large-scale diffraction-110

based and the fine-scale reflection-based estimates.

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The paper proceeds as follows. We begin by describing the methodological background of the proposed velocity estimation method. Next, we show the application of our method to two synthetic datasets, which differ in their degree of complexity and realism. Finally, we apply the proposed approach to common-offset 100-MHz GPR field data acquired at the Boise Hydrogeophysical Research Site (BHRS) near Boise, Idaho, USA.

118

119 **2 Methodology**

We assume in our work that the subsurface velocity distribution v(x, z) can be regarded as the sum of a smoothly varying or constant background velocity field $v_0(x, z)$ and a smallscale velocity fluctuation field $\Delta v(x, z)$ (e.g., Pullammanappallil et al. 1997; Poppeliers 2007; Irving et al. 2009; Scholer et al. 2010)

$$v(x,z) = v_0(x,z) + \Delta v(x,z). \tag{1}$$

To determine v(x, z) from a common-offset GPR reflection dataset, we separate the recorded 124 wavefield into its diffracted and reflected components, which are used to estimate v_0 and Δv , 125 respectively. This inherently assumes that the background velocity field is smooth at the scale 126 of a dominant GPR wavelength and beyond, such that it does not contribute to the reflected 127 wavefield. Figure 1 illustrates schematically the steps involved in our velocity estimation 128 procedure. First, diffractions are separated and analyzed in order to infer the spatially variable 129 RMS and interval velocity structures. The latter serves as v_0 , whereas the former is used to 130 migrate the common-offset GPR data, after which the dominant reflections are separated. 131

Assuming a convolutional relationship between the velocity perturbation field and the reflection data based on an estimated mixed-phase wavelet, a L1-norm constrained inversion is then used to infer Δv . Below we describe in detail this inversion workflow in terms of the following four main components: (i) diffraction separation, (ii) background velocity estimation, (iii) reflected wavefield prediction, and (iv) velocity perturbation inversion.

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138 **2.1 Diffraction separation**

The diffracted wavefield is obtained in our methodology via plane-wave destruction (PWD) filtering (Fomel, 2002). The underlying assumption when using this approach is that reflections correspond primarily to coherent events having slowly changing slopes in the *x*-*t* domain, whereas the slopes associated with diffractions are significantly more spatially variable. The goal of PWD filtering is to destroy locally planar events in the data corresponding to an estimated slope field $\sigma(x, t)$. By regularizing the estimation problem, it is possible to destroy only those events whose slopes change slowly in space, thereby isolating the diffracted energy.

147 A local plane wave in the *x*-*t* domain can be expressed by the following differential equation 148 (e.g., Fomel, 2002):

$$\frac{\partial u}{\partial x} + \sigma \frac{\partial u}{\partial t} = 0, \tag{2}$$

149 where u(x, t) is the wavefield and σ is the local slope. If the local slope in a seismic or GPR 150 dataset is unchanging in time, the wavefields observed at two adjacent trace positions x_i and 151 x_{i+1} are related by a time shift $\sigma \Delta x$, where Δx is the trace spacing. That is,

$$u(x_{i+1},t) = u(x_i,t + \sigma \Delta x), \tag{3}$$

152 which has the Fourier transform

$$U(x_{i+1},\omega) = U(x_i,\omega)e^{i\omega\sigma\Delta x}.$$
(4)

Equation (4) shows that we can predict the trace at position x_{i+1} from the trace at position x_i by application of a linear phase shift. To apply this concept to data with temporally variable local slopes, Fomel (2002) used the fractional delay filter of Thiran (1971) to derive a localized, discrete, time-domain approximation to $e^{i\omega\sigma\Delta x}$ whose coefficients depend nonlinearly on the local slope values. Prediction of a trace using its neighbor can then be accomplished by matrixvector multiplication

$$\mathbf{u}_{i+1} = \mathbf{P}_{i,i+1}\mathbf{u}_i,\tag{5}$$

where $\mathbf{P}_{i,i+1}$ is a time-variable convolution matrix linking trace vectors \mathbf{u}_{i+1} and \mathbf{u}_i , whose entries are a nonlinear function of the local slope field $\sigma(x, t)$.

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The PWD problem seeks to estimate $\sigma(x, t)$ by minimizing the prediction error for an entire seismic or GPR section, thereby destroying the local plane waves in the data. Considering the section **s** as a column vector containing all of the traces, i.e., $\mathbf{s} = [\mathbf{s}_1^T \mathbf{s}_2^T \dots \mathbf{s}_n^T]^T$, this is described by

$$\mathbf{r} = \mathbf{D}\mathbf{s},\tag{6}$$

where \mathbf{r} is the destruction residual, and \mathbf{D} is the destructor matrix defined by:

$$\mathbf{D} = \begin{bmatrix} -\mathbf{P}_{1,2} & \mathbf{I} & 0 & \cdots & 0\\ 0 & -\mathbf{P}_{2,3} & \mathbf{I} & \cdots & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & \cdots & 0 & -\mathbf{P}_{n-1,n} & \mathbf{I} \end{bmatrix},$$
(7)

167 with I representing identity operator. The estimation of $\sigma(x,t)$ is accomplished via

regularized nonlinear least-squares minimization of equation (6), where shaping regularization 168 (Fomel 2007a) is used to control the smoothness of the estimated slope field. In our case, the 169 considered lateral smoothing radius for the regularization must be large enough to estimate a 170 slope field that well represents the reflections in the dataset, but not the diffractions. The 171 prediction residual corresponding to the estimated slope field is simply the GPR section with 172 the reflection events removed. All of the above steps are performed in our work using the 173 programs 'sfdip' and 'sfpwd' in Madagascar (https://reproducibility.org/), an open-source data 174 analysis package. 175

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177 2.2 Background velocity estimation

Once the diffracted wavefield has been separated, the next step is to use it to estimate the lowfrequency background velocity field v_0 , which, due to its smoothness at the wavelength scale, does not to contribute to the reflected wavefield. To this end, we first estimate the RMS velocity distribution by examining the focusing of diffractions during migration using a suite of constant velocity values. Fomel et al. (2007) proposed a migration focusing metric based on local kurtosis, whereas Decker et al. (2017) considered the local semblance attribute. Here, we use the latter measure, which can be defined as

$$s(x,t,v) = \frac{\left(F_{v}(a(x,t))\right)^{2}}{F_{v}(a^{2}(x,t))},$$
(8)

where a(x,t) denotes the diffraction amplitude as a function of horizontal position x and time t, and operator F_v denotes time migration using constant velocity v. Migration is performed on both the diffracted wavefield and its square using the velocity continuation

method of Fomel (2003), which results in two space-time-velocity cubes. In Madagascar, this 188 step is accomplished using the program 'sfvelcon'. The division in equation (8) is then 189 performed in a regularized manner using the program 'sfdivn' in order to constrain the 190 smoothness of the resulting local semblance cube (Fomel, 2007b). Using the automatic picking 191 algorithm 'sfpick' (Fomel, 2009), the maxima on each time-velocity panel are next selected, 192 which yields a 1D RMS velocity curve at each trace location. These curves are combined into 193 a 2D RMS velocity model, which is finally provided as input to the constrained Dix inversion 194 program 'sfdix' (Fomel and Guitton, 2006) to estimate $v_0(x, t)$. 195

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197 **2.3 Reflection separation**

In order to obtain the reflected wavefield that is used in our inversion procedure to estimate the 198 velocity perturbation Δv , two steps are performed. First, the GPR profile is time-migrated 199 based on the inferred RMS velocity model from Section 2.2 using the velocity continuation 200 method described in Fomel (2003). This has the effect of collapsing diffractions and moving 201 dipping reflectors to their correct positions in terms of vertical traveltime, and is accomplished 202 using the Madagascar programs 'sfvelcon' and 'sfslice'. Then, we apply the PWD method to the 203 migrated reflection section in order to estimate the local slopes, which in this case are used to 204 predict the time-migrated reflected wavefield void of migration artifacts and random noise 205 (Fomel and Guitton, 2006). The latter step is accomplished using the Madagascar program 206 'sfpwdsmooth2'. Note that our use of PWD here is different compared to what was presented 207 in Section 2.1, where the method was used to suppress reflected energy in the data and isolate 208 the diffracted wavefield. In this regard, it is important to note that a high-quality reflection 209

section cannot be obtained by simply subtracting the diffracted wavefield from the GPR data.
Indeed, predicting the reflected wavefield from the estimated slopes of the time-migrated
image results in a cleaner section that is much more amenable to the velocity perturbation
inversion described next.

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215 **2.4 Velocity perturbation inversion**

To estimate the velocity perturbation field Δv , we perform sparse inversion of the timemigrated reflected GPR wavefield obtained in Section 2.3. To this end, we assume that the wavefield can be effectively described using the so-called primary reflectivity section (PRS) model (e.g., Gibson and Levander, 1990; Holliger et al., 1994; Irving et al., 2009), whereby the time-migrated data, d(x,t), are expressed as the convolution product of the GPR source wavelet, w(t), and the subsurface reflectivity distribution, r(x,t)

$$d(x,t) = w(t) * r(x,t).$$
 (9)

Equation (9) is well known to provide an adequate model for zero-offset seismic or GPR 222 reflection data when single scattering prevails and dispersion is absent (e.g., Yilmaz, 2001). P 223 Although the second assumption is only strictly valid for GPR data acquired in perfectly 224 electrically resistive environments, experience has shown that this model is able to 225 accommodate the limited dispersion effects linked to low-loss conditions for which the GPR 226 method is suitable (e.g., Irving et al., 2009; Xu et al., 2020). Indeed, such effects in GPR data 227 tend to be inherently rather minor, as it is simply impossible to acquire high-quality GPR 228 reflection data in strongly dispersive environments. 229

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As the subsurface reflectivity can be approximated using the temporal derivative of the velocity perturbation field (e.g., Pullammanappallil et al. 1997; Poppeliers 2007), and because the temporal derivative operator may be treated as a finite-difference filter whose position within a convolution equation can be shifted (Irving et al. 2009; Scholer et al. 2010), equation (9) leads to

$$d(x,t) \approx w(t) * \frac{\partial}{\partial t} \Delta v(x,t)$$

= $g(t) * \Delta v(x,t)$, (10)

where g(t) represents the time-differentiated GPR wavelet. Expression (10) provides a linear relationship between the time-migrated reflected GPR wavefield and the velocity perturbation field, which forms the basis for our inversion procedure. Indeed, considering data vector **d** containing all of the GPR traces arranged into a single column, i.e., $\mathbf{d} = [\mathbf{d}_1^T \mathbf{d}_2^T \dots \mathbf{d}_n^T]^T$, and model vector **m** containing the corresponding velocity perturbations underlying each trace arranged into a single column, i.e., $\mathbf{m} = [\Delta \mathbf{v}_1^T \Delta \mathbf{v}_2^T \Delta \mathbf{v}_3^T \dots \Delta \mathbf{v}_n^T]^T$, we have

$$\mathbf{d} = \mathbf{G}\mathbf{m},\tag{11}$$

where **G** is a block-diagonal matrix containing *n* replicates of the convolution matrix associated with the time-differentiated wavelet g(t).

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To define the kernel matrix **G**, information on the GPR source wavelet is required. In this work, we estimate w(t) from the reflected wavefield using the method of Schmelzbach & Huber (2015), which assumes that a typical mixed-phase GPR source wavelet can be considered as a minimum-phase wavelet that has been shifted by a constant phase angle. To first estimate the corresponding minimum-phase wavelet, we perform standard least-squares spiking deconvolution on the reflected wavefield and take the inverse of the deconvolution operator (e.g., Buttkus, 2000). A search of the phase rotation angle that maximizes the kurtosis when applied to this minimum-phase wavelet is then used to obtain the final mixed-phase GPR source wavelet. The practical validity of this source wavelet estimation procedure was recently demonstrated by Xu et al. (2021). Note that the effects of minor dispersion in the GPR data are, at least in part, accounted for in the sense that an effective wavelet that best fits the considered dataset in its entirety, rather than the true emitted GPR source signal, is estimated.

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To invert for the velocity perturbation \mathbf{m} given the reflection data \mathbf{d} , we minimize the following objective function

$$\theta(\mathbf{m}) = \|\mathbf{G}\mathbf{m} - \mathbf{d}\|_2^2 + \lambda \|\mathbf{D}\mathbf{m}\|_1, \tag{12}$$

where $\|\cdot\|_p$ denotes the L-p norm, λ is a trade-off parameter that controls the desired balance between fitting the data and honoring the prescribed prior information about the model, and matrix **D** is given by

$$\mathbf{D} = \begin{bmatrix} \mathbf{D}_{\mathrm{x}} \\ \alpha \ \mathbf{D}_{\mathrm{t}} \end{bmatrix}. \tag{13}$$

Here, $\mathbf{D}_{\mathbf{x}}$ and $\mathbf{D}_{\mathbf{t}}$ are finite-difference matrices that approximate the first derivatives of the velocity perturbation model in the horizontal and temporal directions, respectively, and α is an anisotropy parameter that controls the degree of desired smoothing between the temporal and horizontal directions. The choice of α should reflect the expected aspect ratio of the underlying GPR velocity heterogeneity.

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Equation (12) corresponds to a regularized least-squares inversion with blocky model prior constraints. That is, in seeking to minimize the L1-norm of the first derivatives of the velocity

perturbation field, we tend to recover models that have a sparse first derivative structure, 271 meaning a piecewise-constant or blocky appearance. Note that this approach has similarities to 272 sparse spike deconvolution in seismic data processing, which uses sparsity constraints to 273 recover the underlying reflectivity series from a seismic trace (e.g., Claerbout and Miur, 1973; 274 Oldenburg et al., 1983; Velis, 2008). Our method differs, however, in the sense that (i) we use 275 sparsity applied to the first derivative of the velocity perturbation field and invert for the latter 276 directly, rather than inverting for a sparse reflectivity series; and (ii) we invert all traces at once 277 with both vertical and lateral regularization constraints in order to estimate the full 2D velocity 278 perturbation field. 279

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Due to the presence of the L1-norm, the minimization of equation (12) is nonlinear. To address this, we use an iteratively reweighted least squares (IRLS) approach based on the following approximation of the Lp-norm proposed by Ekblom (1973):

$$\|\mathbf{x}\|_{p} \approx \sum_{i=1}^{n} (x_{i}^{2} + \epsilon^{2})^{p/2},$$
 (14)

where ϵ is a small user-defined value (e.g., Farquharson and Oldenburg, 1998). Taking the derivative of equation (12) with respect to **m** and setting it to zero, and considering approximation (14), we arrive at

$$(2\mathbf{G}^{\mathrm{T}}\mathbf{G} + \lambda \mathbf{D}^{\mathrm{T}}\mathbf{R}\mathbf{D}) \mathbf{m} = 2\mathbf{G}^{\mathrm{T}}\mathbf{d}, \qquad (15)$$

287 where

$$\mathbf{R}_{ii} = \frac{1}{|(\mathbf{D}\mathbf{m})_i| + \epsilon} \tag{16}$$

is a diagonal reweighting matrix. We solve for **m** iteratively as follows:

289

290 (1) Set $\mathbf{R} = 2\mathbf{I}$.

291 (2) Solve equation (15) for \mathbf{m} using the conjugate gradient method.

292 (3) Update **R** using equation (16) and the result for **m** obtained in Step 2.

(4) Return to Step (2) and iteratively update **m** until a defined maximum number of iterations
or desired data fit is reached.

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In carrying out the above steps, the first iteration of our inversion procedure solves for the velocity perturbation field corresponding to an L2-norm constraint on the model derivative term in equation (12). This and subsequent solutions are then used within the IRLS reweighting scheme in order to gradually converge to the L1-norm solution, typically within a few iterations. Once $\Delta v(x, t)$ has been obtained, it is added to the estimated background velocity model $v_0(x, t)$ from Section 2.2. As a final step, the resulting subsurface velocity field in terms of vertical two-way traveltime, v(x, t), is converted to depth to obtain the desired v(x, z).

304 **3 Results**

305 3.1 Application to synthetic data

In the following, we test and validate the velocity estimation technique outlined in Section 2 and illustrated in Figure 1 by applying it to synthetic common-offset GPR reflection data. We first consider a layered subsurface velocity model containing a small number of well-defined point-type diffractors. We then move to an arguably more realistic scenario involving a stochastic velocity distribution characterized by the explicit absence of idealized diffracting 311 structures.

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313 <u>3.1.1 Layered model</u>

Our layered velocity model, which is shown in Figure 2a, is similar to that recently considered 314 by Yuan et al. (2019) in a diffraction imaging study. The model contains two main velocity 315 units separated by a dipping interface. A thin horizontal bed, with a thickness of 0.5 m, is 316 present in the underlying unit. Both the upper and lower units contain three circular diffractors 317 with diameters ranging from 0.4 to 0.6 m. The corresponding relative dielectric permittivities 318 of the upper and lower layers, the thin bed, and the diffractors are 9, 16, 25, and 4, respectively. 319 The electrical conductivity of all materials is fixed at a constant value of 1 mS/m, and the 320 magnetic permeability is assumed to be equal to its value in free space. 321

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Synthetic common-offset GPR reflection data were simulated over the layered velocity model 323 using the gprMax software (Warren et al. 2016), which solves Maxwell's equations using the 324 finite-difference time-domain (FDTD) method. The transmitter and receiver antennas, which 325 are approximated by point electric dipoles, were spaced 0.5 m apart and moved at 0.1 m 326 increments along the survey profile. The source antenna current function was specified as a 327 Ricker wavelet having a dominant frequency of 100 MHz, which resulted in a propagating 328 electromagnetic pulse corresponding to the first derivative of this function. The resulting 329 synthetic GPR data were then contaminated with 2% Gaussian random noise (Figure 2b) prior 330 to being subjected to a standard processing flow involving (i) elimination of the direct air and 331 ground arrivals from the data by subtracting the average trace calculated over a time window 332

from 0 to 36 ns using a moving spatial window of 50 traces; (ii) amplitude scaling to compensate for energy spreading, absorption, and scattering using a gain function of the form $g(t) = (1 + at)e^{bt}$; and (iii) 5-300 Hz bandpass filtering. With time measured in nanoseconds, the parameters a and b were chosen empirically to be 0.3 ns⁻¹ and 0.2 ns⁻¹, respectively, such that the gain function brought all amplitudes along a given trace to the same average level. Figure 3a shows the resulting unmigrated processed data section.

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Following the velocity estimation workflow outlined in Section 2 and illustrated in Figure 1, 340 diffractions were first separated from the processed data using PWD filtering (Figure 3b). The 341 diffracted wavefield was then subjected to velocity continuation and local kurtosis analysis in 342 order to estimate the RMS velocity structure (Figure 3c), which was used in a Dix inversion 343 procedure to obtain the low-frequency background velocity field diplayed in Figure 3d. Note 344 that this result shows some resemblance to the underlying model in Figure 2a. However, it fails 345 to adequately represent the dipping interface as a sharp discontinuity having a constant slope, 346 and it entirely misses the thin bed. In Figure 3e, we show the GPR reflection data after time 347 migration based on the estimated RMS velocity structure in Figure 3c. We see that the data 348 have been adequately imaged apart from some residual "smiles", which are attenuated through 349 the application of PWD to isolate the specular reflections (Figure 3f). From the separated 350 reflection image, a mixed-phase GPR wavelet was estimated (Schmelzbach & Huber 2015), 351 which is compared with the first derivative of the Ricker source current function in Figure 3g. 352 Figure 3h shows the velocity perturbation field inferred through our L1-norm inversion 353 approach using a value of $\alpha = 10$ and after 5 IRLS iterations. We observe that the high-354

frequency elements present in Figure 2a have now been estimated, but not the low-frequency 355 velocity trend. Finally, Figures 3i and 3j show the complete estimated velocity model, equal to 356 the sum of the background and perturbation fields, in terms of two-way traveltime and after 357 conversion to depth, respectively. The comparison with the reference velocity model (Figure 358 2a) is quite favorable, which clearly illustrates the potential benefits of the proposed 359 diffraction- and reflection-based velocity estimation approach. In this context, is important to 360 emphasize that the former can only resolve the smooth large-scale velocity structure and, hence, 361 entirely misses the presence of the thin bed (e.g., Yuan et al. 2019) whereas, on its own, the 362 latter requires coincident borehole information for calibration and recovery of the large-scale 363 component of the velocity structure (e.g., Schmelzbach et al. 2012; Xu et al. 2021). 364

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366 <u>3.1.2 Heterogeneous model</u>

We now test our proposed methodology on an arguably more realistic model of the shallow subsurface. In this regard, we consider the stochastic velocity distribution shown in Figure 4a, which is meant to emulate a heterogeneous surficial alluvial environment. The model was geostatistically generated based on the von Kármán autocorrelation function, which describes a band-limited fractal medium (e.g., Tronicke & Holliger 2005) and is given by

$$C(r) = \frac{r^{\nu} K_{\nu}(r)}{2^{\nu - 1} \Gamma(\nu)},$$
(17)

where $K_{\nu}(r)$ is the modified Bessel function of the second kind of order $0 \le \nu \le 1$, Γ is the gamma function and

$$r = \sqrt{(x/a_x)^2 + (z/a_z)^2}$$
(18)

is the weighted radial autocorrelation lag with a_x and a_z denoting the correlation lengths

along horizontal and vertical directions x and z, respectively. Values of v = 0.5, $a_x = 2.0$ m, and $a_z = 0.2$ m were considered, along with a mean velocity of 0.1 m/ns and a standard deviation equal to 0.01 m/ns. The generated multi-Gaussian velocity realization was then transformed into a facies-type distribution through thresholding, whereby six units having constant velocities equal to 0.079, 0.092, 0.100, 0.105, 0108, and 0.116 m/ns were specified.

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To generate synthetic common-offset GPR reflection data over the velocity model in Figure 4a, 381 we again used the gprMax software (Warren et al. 2016). Velocity values v were converted to 382 relative dielectric permittivity ε for the FDTD modeling using the low-loss approximation 383 $v \approx 1/\sqrt{\varepsilon\mu}$, where the magnetic permeability μ was assumed equal to its value in free space. 384 As was done previously, the electrical conductivity was fixed at a constant value of 1 mS/m. 385 For the source antenna current function, we considered for this simulation the derivative of a 386 Blackman-Harris window having a dominant frequency of 100 MHz (Irving and Knight, 2006). 387 The spacing between the transmitter receiver antennas was again set to 0.5 m, and traces were 388 simulated every 0.1 m along the profile. Figure 4b shows the resulting synthetic GPR data with 389 the addition of 2% Gaussian noise. Processing of these data was essentially identical to that for 390 the layered synthetic velocity model except that the averaging window used for the first-arrival 391 removal was set from 0 to 25 ns, and the gain parameters a and b were set to 0.2 ns⁻¹ and 392 0.2 ns⁻¹, respectively. The processed GPR section is shown in Figure 5a. 393

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Figure 5b shows the diffracted wavefield estimated from the processed data in Figure 5a, which was used to infer the RMS velocity structure (Figure 5c) and, subsequently, the background

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velocity field through Dix inversion (Figure 5d). In Figure 5e, we show the time-migrated GPR 397 section based on the RMS velocity field, from which the reflected wavefield was obtained 398 (Figure 5f). The latter was used to estimate an effective mixed-phase source wavelet, which is 399 shown in Figure 5g and seen to compare favorably to the true source wavelet corresponding to 400 the derivative of the considered input current function. Finally, in Figures 5h, 5i, and 5j, we 401 show the inverted velocity perturbation field obtained after 5 IRLS iterations using a value of 402 $\alpha = 10$, along with the final estimated velocity model in terms of two-way traveltime and depth, 403 respectively. Comparison of Figure 5j with the underlying velocity model in Figure 4a 404 demonstrates remarkably good agreement, but also points to two interesting aspects of the 405 proposed velocity estimation method that did not become evident in its application to the more 406 idealized layered model (Figures 2 and 3). The first concerns the influence of the direct wave 407 and its muting, which, in the presence of small-scale heterogeneity, inherently affects the 408 viability and accuracy of the velocity estimation over a depth range corresponding to 409 approximately one dominant wavelength, that is, the first ~1 m depth. The second observation 410 concerns the importance of the background velocity model and its impact on the final result. 411 This is illustrated by the fact that our final velocity model (Figure 5j) misses the pervasive low-412 velocity zone between ~ 2 and ~ 3.5 m depth in the central and right-hand side of the model 413 from \sim 7 m to \sim 20 m lateral distance, which can be directly related to the limited resolution of 414 the estimated background velocity model. 415

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417 **3.2 Application to field data**

418 <u>3.2.1 Database</u>

We now apply the proposed velocity estimation method to a field GPR dataset acquired at the 419 Boise Hydrogeophysical Research Site (BHRS). The BHRS is a research wellfield located on 420 a gravel bar adjacent to the Boise River near Boise, Idaho, USA (Figure 6). The surficial aquifer 421 consists of late Quaternary fluvial deposits dominated by gravel and sand, and is underlain by 422 a layer of red clay at ~20 m depth (Barrash & Clemo 2002). The depth of the groundwater table 423 at the site varies seasonally between ~ 2 m and ~ 4 m. Over the past two decades, the BHRS has 424 been extensively utilized for the testing, validation, and improvement of a wide variety of 425 geophysical and hydrogeological characterization methods (e.g., Tronicke et al. 2004; Bradford 426 et al. 2009; Dafflon et al. 2009, 2011; Hochstetler et al. 2016; Xu et al. 2020, 2021). 427

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The considered common-offset, bi-static GPR reflection prosfile is a part of 3D survey 429 performed at the BHRS in 1998 using a Pulse Ekko Pro 100 system (Sensors & Software Inc.) 430 with 100 MHz nominal center frequency antennas, and can be considered as a reference for 431 surface-based GPR reflection data collected in alluvial environments (e.g., Xu et al., 2020, 432 2021). The profile has a length of 30 m and crosses three boreholes, B5, A1, and B2, for which 433 neutron-neutron porosity logs are available below the groundwater table (Figure 6). While the 434 exact values have not been reported, the depth of the latter at the time of acquisition of the GPR 435 data and neutron-neutron logs was approximately 2 m. The GPR data were collected using a 436 constant antenna spacing of 1 m, a lateral trace increment of 0.1 m, and a time sampling interval 437 of 0.8 ns. For each recorded trace, 32 stacks were performed to improve the signal-to-noise 438

ratio. Antenna positioning errors and differences in antenna coupling across the profile were
estimated to be negligible. Figure 7 shows the GPR reflection section after minor preprocessing.

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443 <u>3.2.2 Velocity estimation</u>

The considered field GPR data were subjected to a processing flow consisting of, in order, 444 time-zero correction, DC shift removal, "de-wow" filtering, removal of the direct air and 445 ground arrivals, correction for the antenna offset, and amplitude scaling. Time-zero was 446 determined based on the first deflection of the data above the ambient noise level. While 447 slightly different approaches are possible, we estimate that the corresponding uncertainties do 448 not exceed ~ 2 ns. To correct for antenna offset, we used the average velocity of the vadose 449 zone of 0.14 m/ns inferred from previous work (e.g., Bradford, 2008; Bradford et al., 2009). 450 Contrary to our synthetic examples which involved an antenna spacing of 0.5 m, correction for 451 the larger offset between the antennas in the case of the BHRS data was deemed necessary and 452 should lead to negligible differences in traveltime beneath the direct air and ground arrivals 453 compared to the corresponding zero-offset acquisition. Due to the proximity of the direct 454 arrivals to the reflection from the groundwater table, we used a manual surgical mute to remove 455 them as opposed to the average trace subtraction technique considered previously. As was done 456 for the synthetic data, amplitude scaling was performed using a gain function of the form 457 $g(t) = (1 + at)e^{bt}$, where the parameters a and b that best balanced the amplitudes along 458 any given trace were found to be 0.5 ns⁻¹ and 0.8 ns⁻¹, respectively. It is important to emphasize 459 that, with this choice of gain function that smoothly varies in time, the relative reflection 460

amplitudes along the GPR traces are importantly well preserved, which would not be the casewith the use of an AGC-type amplitude scaling.

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Figure 8a shows the processed GPR section, to which we then applied the proposed velocity 464 estimation methodology. Following the workflow described in Section 2 and illustrated in 465 Figure 1, we began with the separation of the diffractions (Figure 8b) which, although not 466 evident in the original processed data, turn out to be quite abundant, particularly in the central 467 part of the profile. This was followed by the estimation of the RMS velocity structure (Figure 468 8c) and subsequent Dix inversion to infer the background velocity field (Figure 8d). The latter 469 points to the presence of a rather prominent low-velocity zone at intermediate depths in the 470 left-hand side of the profile. The inferred RMS velocity structure was then used to perform 471 time-migration of the GPR section (Figure 8e) which, overall, appears to result in an adequate 472 focusing and imaging of the data. An exception are the artefacts introduced into the uppermost 473 part of the section, which are likely related to the harsh surgical muting of the direct wave as 474 well as its potential interference with the neighboring reflection from the groundwater table. 475 Figure 8f shows the reflected wavefield that was extracted from the migrated section, which 476 we see to be largely devoid of these artefacts. After estimating the effective mixed-phase source 477 wavelet (Figure 8g) using the method of Schmelzbach and Huber (2015), we proceeded to 478 invert the imaged reflected wavefield for the underlying velocity perturbations using a value 479 of $\alpha = 10$, whose choice was based on the typical aspect ratio encountered in similar 480 heterogeneous environments as well as previous BHRS studies (Gelhar, 1993; Xu et al., 2020, 481 2021). The results, which are shown in Figure 8h, clearly depict the dramatic velocity 482

discontinuity associated with the groundwater table. Finally, Figures 8i and 8j show the superposition of the large-scale background velocity structure (Figure 8d) and the inverted small-scale velocity perturbation field (Figure 8h) in terms of two-way traveltime and depth, respectively. Note that in deriving the latter, we also accounted for some mild topographic variations that were present along the profile. Note that, in the case fo significant topographic variations, such variations would need to be corrected for earlier in our analysis procedure.

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Although the inferred velocity distribution presented in Figure 8j is clearly dominated by the 490 sharp transition from high to low velocities across the water table, the underlying saturated 491 zone shows a significant degree of velocity heterogeneity. This heterogeneity largely emulates 492 the structure depicted by the reflected wavefield in Figure 8d and, as such, is geologically 493 plausible. To further assess the realism of our results, we compare them with the neutron-494 neutron porosity logs available in the saturated zone for boreholes B5, A1, and B2 (Figure 6). 495 To this end, we transform the porosity logs to GPR velocity v using a standard petrophysical 496 mixing model (e.g., Huisman et al. 2003) 497

$$\nu = \frac{c}{\sqrt{\varepsilon_r^s}(1-\phi) + \sqrt{\varepsilon_r^w}\phi'},\tag{19}$$

where c = 0.3 m/ns is the speed of light in free space, ϕ is the porosity, and $\varepsilon_r^s = 4.6$ and $\varepsilon_r^w = 80$ are the relative dielectric permittivities of the dry solid matrix and water, respectively. A relative dielectric permittivity of 4.6 for the dry matrix corresponds to the average value for quartz (e.g., Schön, 2015) and, as such, is widely regarded as being suitable for alluvial environments in general and the BHRS in particular. Indeed, Dafflon et al. (2009) demonstrated the overall suitability of a relative dielectric permittivity of 4.6 for the solid matrix at the BHRS. While variations in this parameter on the order of 10 to 15% are conceivable, the associated uncertainties are minor and, hence, largely irrelevant compared to other sources of uncertainty in our inversion results and the neutron-neutron logs.

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Figure 9 shows the comparison between the GPR-derived velocity and the converted porosity 508 logs at the borehole locations. Overall, we see that the curves are in good agreement, not only 509 in terms of the trend, but also with regard to the absolute values. In this context, it is important 510 to note that the inferred velocity estimates are at least as accurate as those previously inferred 511 from multi-offset GPR reflection tomography (Bradford et al., 2009), while at the same time 512 exhibiting a significantly higher resolution. Arguably, the most conspicuous mismatch between 513 the GPR- and neutron-neutron-based velocity profiles is a seemingly systematic depth shift of 514 \sim +0.5 m of the former with regard to the latter, which was recently discussed by Xu et al. 515 (2021). This could be related to the depth calibration of the neutron-neutron logs and/or to a 516 systematic overestimation of the GPR velocity in the vadose zone, the latter of which is the 517 most poorly constrained part of our inferred velocity model due to partial interference between 518 the direct arrivals and the reflection from the water table. Conversely, this apparent mismatch 519 is unlikely to be related to the time-zero determination, whose uncertainty is estimated to be 520 on the order of 2 ns. 521

522

523 4 Discussion and Conclusions

524 We have presented in this paper a novel method for estimating the detailed high-frequency 525 electromagnetic velocity distribution in the shallow subsurface from surface-based common-

offset GPR reflection data. The smooth background component of the velocity structure is 526 estimated from the diffracted part of the recorded wavefield, whereas the superimposed small-527 scale fluctuations are inferred from the associated reflected component. An important and 528 distinguishing feature of our methodology is that, in contrast to previous related approaches 529 (e.g., Schmelzbach et al. 2012; Liu et al. 2018; Xu et al. 2021), it does not require any borehole 530 calibration and/or conditioning information. It does, however, inherently rely upon the 531 presence of diffractions in the GPR data. In this regard, it is important to note that, although 532 diffractions are often not immediately obvious in a GPR profile, they can become much more 533 evident after wavefield separation. This is clearly illustrated in Figure 8. 534

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The proposed technique was tested and validated on synthetic data corresponding to two 536 velocity models of differing complexity and realism: one an idealized layered model containing 537 a small number of discrete diffractors, and the other a stochastic facies-based model emulating 538 the typical heterogeneity observed in surficial alluvial environments (e.g., Gelhar 1993; 539 Tronicke et al. 2004; Tronicke and Holliger 2005). These synthetic tests not only illustrate the 540 fundamental validity and robustness of our method, but also allow us to identify a number of 541 features that merit attention during its application. Successful validation of our approach on the 542 BHRS field data further illustrates its capacity for estimating complex velocity structures. 543

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Results for our synthetic test involving the stochastic subsurface model (Figures 4 and 5) showed a loss of accuracy in the shallowest part of the inferred velocity distribution due to the elimination of the direct air and ground arrivals, which removed important reflections from this

zone. Processing techniques used for this purpose, such as subtracting the average trace in a 548 corresponding time window, will thus affect the inferred velocity model over an initial depth 549 range of roughly 1-2 dominant wavelengths (Figures 4 and 5). Another interesting feature 550 emerging from the stochastic synthetic example is the fact that we fail to fully resolve the thin 551 low-velocity zone between ~ 2 m and ~ 3.5 m depth, notably in the central and right-hand side 552 of the profile. A bias in the estimated background velocity distribution over these depths 553 (Figure 5d) is likely the cause of this result. Given that this region has a density of diffractions 554 that is comparable to the rest of the model, this may point to the inherently limited resolution 555 of the inferred background velocity field. Under ideal circumstances, diffraction-based velocity 556 analysis can be expected to achieve a resolution on the order of one dominant wavelength, 557 which for the considered synthetic data is of the order of ~ 1 m. In practice, however, the 558 achievable resolution critically depends on the so-called smoothing radius parameter, which 559 controls the regularization of a number of steps in the diffraction velocity analysis procedure 560 (Fomel et al., 2007). As recently illustrated by Yuan et al. (2019), a smoothing radius that is 561 too small leads to unstable estimates of the diffraction-derived velocity model, whereas one 562 that is too large will lower unnecessarily its resolution. While we made every effort to 563 determine an optimal value of the smoothing radius for all data considered in this study, there 564 may be regions in the final velocity model where the large- and small-scale components 565 inadequately complement each other due to the limited resolution of the former. 566

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Arguably, the most important criterion that must be fulfilled for our method to perform satisfactorily is the presence of an ample amount evenly distributed diffractions throughout the

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recorded constant-offset GPR section. Given the inherent heterogeneity of the shallow 570 subsurface (e.g., Gelhar, 1993; Hubbard and Rubin, 2005; Dafflon et al., 2009; Xu et al., 2021), 571 this condition is likely to be fulfilled even if the diffracted energy is not directly obvious in the 572 original recorded data (Figures 5 and 8). Nonetheless, in the case where an sufficient amount 573 of diffracted energy cannot be retrieved through wavefield separation and/or where the 574 diffraction events are highly unevenly distributed throughout the probed subsurface region, 575 standard common-midpoint-type analyses may still be used to estimate the large-scale velocity 576 structure with our methodology. Under these circumstances, only the estimation of the 577 background field would change, and the inversion for the small-scale velocity fluctuations 578 would remain the same. 579

580

Two final assumptions upon which our method relies are that the recorded GPR wavefield is 581 largely non-dispersive and is dominated by single scattering. This allows us to use a 582 convolutional model to describe the reflection data, which in turn permits us to pose the 583 velocity perturbation estimation procedure as a highly efficient linear inverse problem. Limited 584 signal attenuation, and thus limited dispersion, is a prerequisite for acquiring surface-based 585 common-offset GPR reflection data of adequate quality and depth of penetration. The practical 586 validity of this assumption is notably underscored by the success of numerous studies explicitly 587 relying upon an adequate estimation of the GPR source wavelet (e.g., Schmelzbach et al., 2012; 588 Schmelzbach and Huber, 2015; Liu et al., 2018; Xu et al., 2021). While it is theoretically 589 conceivable that there exist environments where multiple scattering becomes sufficiently 590 important in GPR studies, the results of extensive testing of the convolutional model on 591

synthetic and field data suggest that the effects of multiples are largely negligible in near-592 surface environments (e.g., Irving et al., 2009; Schmelzbach et al., 2012; Xu et al., 2020,2021). 593 Indeed, in such environments, the combination of small reflection coefficients and signal 594 attenuation due to conductivity-related losses means that multiply reflected energy is not strong. 595 The latter is consistent with a methodological study involving acoustic waves in strongly 596 heterogeneous environments, where it was found that multiple scattering only becomes 597 important for strong local velocity fluctuations, corresponding to standard deviations of the 598 order of 10% and more, in combination with long propagation paths in excess of ~20 dominant 599 wavelengths (e.g., Holliger, 1997). These conditions are generally not fulfilled for surface-600 based constant-offset GPR reflection data. 601

602

An important characteristic of this work is that the proposed methodology is rather 603 straightforward. After basic processing of the GPR data in MATLAB, wavefield separation, 604 diffraction velocity analysis, and Dix inversion are carried out using the Madagascar software 605 package, which is well-established for this purpose. The subsequent wavelet estimation and 606 L1-norm inversion are then again performed in MATLAB. For all of the datasets considered in 607 this study, the total time required to complete all of the steps in our workflow is on the order 608 of one day. The IRLS inversion procedure itself proved to be stable and to converge to 609 consistent estimates of the velocity perturbation field after approximately five iterations. In 610 practical terms, the latter amounted to less than one minute of CPU time on a modest laptop 611 computer. Finally, the inherent computational efficiency of the convolutional model used in 612 our approach implies that the extension of the proposed method to 3D is conceptually 613

straightforward. The only challenge that we anticipate in this regard is the still somewhat
limited practical maturity of 3D diffraction velocity analysis techniques (e.g., Merzlikin et al.
2017; Bauer et al., 2020). A direct benefit of 3D analysis is that errors introduced into the
background velocity estimation procedure by out-of-plane diffractions can be avoided.

618

619 Acknowledgements

Yu Liu gratefully acknowledges financial support of this work through the China Scholarship Council (CSC grant number 201806320359). The considered GPR field data were collected by Michael Knoll and Warren Barrash as part of the initial BHRS characterization, and were kindly provided to us by John Bradford together with the corresponding neutron-neutron porosity logs.

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626 Data availability

627 The data underlying this article will be shared on reasonable request to the corresponding

628 author.

629

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Figure 1. Flowchart illustrating the proposed method for estimating the detailed subsurface velocity structure from surface-based common-offset GPR reflection data.



Figure 2. a) Layered model velocity with discrete diffractors and b) corresponding synthetic common-offset GPR reflection data with 2% Gaussian random noise added.



Figure 3. Velocity estimation process for the layered synthetic velocity model presented in Figure 2a. From the **a**) processed GPR section, the **b**) diffracted wavefield is separated and used to estimate the **c**) RMS velocity structure. Using Dix inversion, the **d**) low-frequency background velocity field $v_0(x, t)$ is obtained. **e**) Time-migrated GPR section based on the RMS velocity structure, from which the **f**) reflected wavefield is obtained. **g**) Comparison of estimated GPR wavelet with the true source wavelet. **h**) Velocity perturbation field $\Delta v(x, t)$ obtained by inverting the reflected wavefield. The final estimated velocity structure (background+perturbation) is shown in terms of **i**) traveltime and **j**) depth.



Figure 4. a) Stochastic velocity model and **b)** corresponding synthetic common-offset GPR reflection data with 2% Gaussian random noise added.



Figure 5. Velocity estimation process for the stochastic synthetic velocity model presented in Figure 4a. From the **a**) processed GPR section, the **b**) diffracted wavefield is separated and used to estimate the **c**) RMS velocity structure. Using Dix inversion, the **d**) low-frequency background velocity field $v_0(x, t)$ is obtained. **e**) Time-migrated GPR section based on the RMS velocity structure, from which the **f**) reflected wavefield is obtained. **g**) Comparison of estimated GPR wavelet with the true source wavelet. **h**) Velocity perturbation field $\Delta v(x, t)$ obtained by inverting the reflected wavefield. The final estimated velocity structure (background+perturbation) is shown in terms of **i**) traveltime and **j**) depth.



Figure 6. Map of the BHRS showing the location of considered common-offset GPR reflection profile (blue dashed line). The profile is aligned with boreholes B5, A1, and B2 (yellow circles).



Figure 7. Common-offset GPR reflection section from the BHRS after minor preprocessing consisting of time-zero correction and "de-wow" filtering.



Figure 8. Velocity estimation process for the BHRS field data presented in Figure 7. From the **a**) processed GPR section, the **b**) diffracted wavefield is separated and used to estimate the **c**) RMS velocity structure. Using Dix inversion, the **d**) low-frequency background velocity field $v_0(x, t)$ is obtained. **e**) Time-migrated GPR section based on the RMS velocity structure, from which the **f**) reflected wavefield is obtained. **g**) Estimated GPR source wavelet. **h**) Velocity perturbation field $\Delta v(x, t)$ obtained by inverting the reflected wavefield. The final estimated velocity structure (background+perturbation) is shown in terms of **i**) traveltime and **j**) depth.



Figure 9. Comparison of the velocity estimated from the common-offset GPR reflection data from the BHRS along boreholes **a**) B5, **b**) A1 and **c**) B2 (black solid lines) with the corresponding converted neutron-neutron porosity logs (blue dashed lines).