Reply to Anonymous Referee # 1 comments

Dear reviewer,
We appreciate your constructive feedback and detailed comments. These have helped to significantly improve the manuscript. We address your comments point-by-point below. Our revised manuscript will cover these aspects.

Sincerely,
Mahtab Rashidifard, Jeremie Giraud, Mark Lindsay, Mark Jessell, Vitaliy Ogarko

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My comments are organized following the paragraph of the paper:

RC1_1: I discover the level-set method with this paper and I had a hard time understanding it from the manuscript. I had then to go through the reading of several papers before entering the manuscript.
On one hand, it's ok, these reading are necessary for learning this method from scratch.
On the other hand, the **method** paragraph of the manuscript turned to be of no help to understand it.

Reply: Thank you very much for listing a very good improvement point here. We were very much pleased to improve the methodology section based on your comments. We agree that the methodology section is not describing the procedure in detail. In the method section, we rely a lot on the given references and on G21 in particular. We have assumed G21 as a compulsory reading and referenced this work several times within the manuscript. However, we have made changes to the theory section in the revised manuscript to make it clearer based on the following detailed comments in this document. These changes can be mainly seen in the method section from lines 79 to 113. We have also added Appendix A to the manuscript which includes required equations for a better understanding of the methodology section.

2.1 **Generalized level-set method**

RC1_2: I thus had two readings of the **summary of the method**. I) Reading as a novice. (that I was), in that case this part is just totally incomprehensible; ii) reading as an expert (that I'm almost now…), the part is still confusing and do not contain the important information. In both cases I felt quite frustrated.

Reply: Thank you for pointing out that the methodology section is not sufficiently explained. Your point is very correct. The level-set method introduced in this paper as is pointed out by the second referee is an adaptation of the generalized level-set approach (by Giraud et al., 2021) for utilising gravity and seismic datasets with different coverage. Thus, in the original submitted manuscript, we didn't go through details in the methodology part. In the revised manuscript, we have taken your suggestions and modified the theory section to make this section more comprehensible.

RC1_3: The authors have the choice, i) either they consider that Giraud et al. 2021 paper (referred below as G21) is a mandatory reading, and then remove the **method summary**, or ii) they give the reader enough material to keep reading the paper before reading G21, if necessary. I think the second solution is the correct one, and without increasing the size, then can give a clear, synthetic description of the problem settings.
I suggest relying on figure 1 that is quite clear and replacing the present method part by:
- Starting with a geometrical description: medium is discretized by cell/nodes (unclear); model is defined by different geological/geophysical units with boundaries (defined on the same mesh); properties are kept constant in geological units; Hence, define N, M, the scope of phi_k
- Boundaries; recall in few words and/or reference level-set and signed distance. A simple drawing showing a 1D phi_k across a boundary with a true versus "smeared" Heaviside would help.
Explain what the authors means by a "multinary structure" or leave that to a reading of G21. I thing that eq. 7 and/or 8 of G21 is worth being recalled here.

Reply: We'd like to thank you for the clear suggested description for the methodology summary section. Selecting option number (ii), with the suggested order, after re-reading the method summary section we find it more graspable. Section 2.1 of the manuscript has been modified based on the three suggested steps above. We have added a new Figure (Fig. A-1) showing the $\boldsymbol{\phi}_k$ across the boundary and also added the smeared Heaviside function equation in Appendix A. We also updated Fig. 1 accordingly for clearer visualisation of the methodology. To avoid confusion, we have deleted the words 'multinary' and leave that detail to the reading of G21.
We have recalled Eq (8) in G21 in the Appendix A as Eq (A4) and briefly elaborate on that from lines 99 to 104 in the revised manuscript.

RC1_4: Setting of the inverse problem. Eq 1 alone can be misleading. It is worth recalling that it comes from a linearization of the problem. I didn't find the information about the iterative scheme that is used to solve the non-linear problem, I guess it's a steepest descent.

Reply: Thank you very much for pointing this detail. We have added information about the iterative scheme in the revised manuscript between lines 101 and 103 With the related reference:
" The system of equations is then dumped into a least-squares system of equations that are solved using the least-square algorithm (Paige and Saunders, 1982). "
This information about the iterative scheme is added before Eq (1) to make it more comprehensible. We have also added a short note about this scheme in the introduction section in the revised version (line 59). Other than that, it has been stated in manuscript (lines 100 and 138) that the system of equations is being solved in least-square framework.
Eq (1) is further updated based on your suggestion in comment No. 9.

Below are some remarks about the text:
RC1_5: 1) You use throughout the text the notion of "rock unit". It seems to me that

"Geological or geophysical unit" would more appropriate since you can deal also with sand, clay, salt, etc.

Reply: After re-examining the text of the original manuscript, we fully agree that using the terms 'geological units', 'lithological unit', 'geophysical units', and 'rock units' in different parts of the manuscript might be confusing. We appreciate you pointing this in your comment. In the revised manuscript we have replaced all other three terms with 'rock unit' as it has been widely used in geoscientific papers as referenced below:
(Giraud et al., 2021b, 2021a; Kieu and Kepic, 2020; Witter et al., 2016, Astic et al., 2020; Lelièvre et al., 2010; Morris et al., 2007). In this study, the defined units are geologically plausible geophysical units so we have replaced all terms with 'rock unit' that covers both concepts.

RC1_6: line 83: you introduce signed-distance values to interface calculated by FMM. Without further explanation, this sentence is totally incomprehensible. Outline is inappropriate, use boundary or interface instead.

Reply: This sentence has been modified along with modifying the methodology summary section based on your comment No. 3. We have provided an illustration of the signed-distance values to the interfaces in the appendix. We have also replaced the word 'outline' with 'boundary' in the revised manuscript. We'd like to thank you for your suggestion.

RC1_7: 2) Line 85: the sentence where you transform a "signed distance" to a multinary structure (???) using a smeared-out Heaviside is obscure.

Reply: We agree that in the original manuscript there was obscurity in the definition of the signed-distance and Heaviside function. The mentioned sentence has now been transformed into clearer sentences along with equations and figures in the appendix.

RC1_8: Line 91-102: This paragraph is very confusing and for me incorrect. The sentence "Initializing the model space…" is confusing. **m()** is the model function that links the modelled data to the parameters, through the signed distance Φ_k . It is not a space, neither in a mathematical sense nor in geometrical sense. And you do not "initialize" a model, unless you talk about the initial (trial) model, you "define" it. You'd rather stick to G21 formulation in this part.

Reply: Thank you for this important remark. We agree that we have used incorrect terms in the manuscript and it was a mistake. In the revised text, we have removed the terms: 'space' and 'initialising' as suggested. We have used your suggested equation (in the following comment) for Eq (1). The entire paragraph and the equation have been modified.

RC1_9: Eq 1 is totally confusing since it mixes a general and an iterative formulation. What is $\mathbf{d}^{calc}$? It is never defined. I suggest to rewrite this paragraph according to a more standard way of presenting inverse problems:
a) You are interested in solving a discrete inverse problem whose direct formulation is:
d=**g**(**m**); **d**= data; **m** parameter to be inverted; **g**() the direct function, non linear in our case.
b) You decide to solve this non linear problem using a gradient type method

base on a 1st order Taylor expansion

$\mathbf{g}(\mathbf{m}) \approx \mathbf{g}(\mathbf{m}0\,) + \frac{\partial g}{\partial \mathrm{m}}\Big|_{m_0} (m - m0\,)$

c) Considering the parameters of your direct problem: **m**=**m**(Φ,ρ) in which density is kept constant, this turns into:

$\mathbf{g}(\mathbf{m}) \approx \mathbf{g}(\Phi 0\,) + \frac{\partial g}{\partial \mathrm{m}} \frac{\partial m}{\partial \Phi}\Big|_{\Phi_0} (\Phi - \Phi_0) \leftrightarrow \mathbf{g}(\mathbf{m}(\Phi)) = \mathbf{g}(\Phi 0\,) + J^{\Phi} \delta\Phi$

d) And you decide to iteratively minimize in a least square sense:

$\Psi_{i+1}^{r} = \|\mathbf{d}^{obs} - g(\Phi_i) - J^{\Phi_i} \delta\Phi\|_2$

where now $\mathbf{d}^{calc} = \mathbf{g}(\Phi_i)$ is defined as the result of the direct problem at iteration i. Please note that compared to your eq1, I have a sign difference. You never use the residuals r that is defined in line94, is it necessary?

Reply: Thanks for writing the step-by-step equations toward linearization of this inverse problem. We consider your commentary about the mathematical notation very appropriate and have accordingly corrected the Eq (1) based on your suggestion. $\mathbf{d}^{calc}$ is now accordingly defined prior to Eq (1). Residuals (r) that encapsulate the difference between calculated and observed datasets are already used in equation 4 so we think it is necessary to keep it and also to be consistent with equations in G21.

RC1_10: 2.2 Regularization level-set inversion

Sentences in lines 118-121 are confusing and the statement is incorrect, this regularization does not "*encourage the* δΦ*update to reach specific values stored in* ***q***", but it does "*encourage the product* ***W***δΦ*update to reach specific values stored in* ***q***" which is quite different (imagine that W is a Laplacian, or a smoothing operator). Since at this point neither **W** nor **q** are defined, it is difficult to understand what the authors mean.

I suggest that the authors replace the text that is too general by more precise details that are given later in the text. What is the exact size of **q** vector?

Do you try to impose something like $\left\| \begin{matrix} W_S \delta\Phi \\ W_P \delta\Phi - \mathrm{v} \end{matrix} \right\|$ minimum?

Reply: Thank you for the suggestion. We corrected the quoted sentence and replaced the general text with more precise details. **W** terms are defined from lines 127 to 130 in the revised text and also in section 2.3. In this case, **W** is not Laplacian or a smoothing operator but weight for regularization terms to encapsulate prior (or constraint in this study) information. We think that your suggested notation is very appropriate so we have deleted the notation **q** and, have taken the suggested formulation as a replacement for Eq (3) in the revised manuscript, as it is more comprehensible.

RC1_11: Besides, why do you mix these two constraints simultaneously?

What is the difference between imposing eq 4 rather than $\|W_S \delta\Phi\| + \|W_P \delta\Phi - \mathrm{v}\|$ minimum? or $\left(\delta\Phi - \delta\Phi_{prior}\right)^T C_{\Phi}^{-1} (\delta\Phi - \delta\Phi_{prior}\,)$?

Should we interpret Wp as a geometrical mask (rather than a weighting) that allows fixing some specific values of boundaries in the different geological units?

Reply: Thank you for your comment. We impose two constraints simultaneously since one of them is applied separately to each unit while the other is a global term. We have added a note on this in the revised manuscript at lines 140-141. The two equations are basically pointing at the same

concept, the only reason we wrote the formulation as Eq (4) is that W_S and $\delta\Phi$ are vectors and the norm might not have a meaning for the product of two vectors. $\|W_S\delta\Phi\| + \|W_P\delta\Phi - \mathrm{v}\|$ can be pointing at the same as Eq (3) in the original manuscript if $\delta\Phi$ is defined as the difference of Φ function between two successive iterations ($\Phi_{k+1} - \Phi_k$) and not as the difference between Φ and Φ_{prior}. However, as was suggested in the previous comment, we have changed the formulation to a closer notation to G21 for more consistency. Eq (3) is changed based on your suggestion and so Eq (4) is now omitted. We have also moved more precise details to the beginning of the paragraph to make the paragraph clearer as was suggested.

As for a reply to the second part of this comment, Wp is interpreted as a weighting term in which geometrical mask can be a particular case of these weights.

RC1_12: 2.3 The sentence on line 149 is incomprehensible, and the full paragraph from 148-153 confusing.

Reply: The entire paragraph is aiming at illustrating the addition of seismic information as a constraint to the inversion. It is using Figure 1 to illustrate. We have slightly updated Fig. 1 in the manuscript and so we updated the corresponding text in the mentioned paragraph for more clarity.

RC1_13: 2.4. Your explanations are ok, however it is difficult to grasp the influence of this topological rule enforcement on your results. Could you comment on the effects of this processing on the synthetic case for instance?

Reply: Thank you for your comment. One example of the effects of applying this topological rule is shown in Fig. 1_1 attached to this document. In this example which is the top view of the unconstrained case (Fig. 5d), it could be seen that the topological rule has reduced the nucleation (inclusion) of the background lithology (blue unit) into the yellow unit. We have added this Figure to the revised manuscript in Appendix B.

RC1_14: 3. Figure 5 caption: what do you mean by difference between "new data and synthetic", what are the new data?

Reply: Thank you for noting this detail. It was a mistake to write 'new data' in the caption. What was meant by new data was, calculated datasets from the final inverted model. It has been corrected now.

RC1_15: 3. A general question: in 4.3 and 4.4 you choose to build a starting model from the inversion of density only, then invert for the interfaces only in a second step. Why don't you try to invert simultaneously for interfaces and density values in the different units?

Reply: Doing the simultaneous inversion for density and interfaces is not a trivial task to do and is not the main focus of this study. Implementing such a technique in the presented level-set study can be a new area of active research that requires the reformulation of the inversion problem. We have added a couple of sentences about this fact to the discussion section from lines 516 to 518 as: "In this area of study, due to lack of availability

of petrophysical datasets we first implement physical properties inversion followed by a constrained level-set inversion. Although simultaneous inversion for density and interfaces would be beneficial to be done in this region, is not a trivial task to do and is beyond the scope of this study".

RC1_16: Line 384: "due to … sections". Use a direct formulation instead: "We present … because…"

Reply: Thanks for the suggestion. The sentence was corrected in the revised text based on your comment.

RC1_17: 4.5.2 I do not understand which geometrical constraints you apply from the seismic profile. On figure 2d for the synthetic case, we clearly see that your constraint follows the geometry of the reflector. What about results obtained on figure 12?
There are no clear reflectors such as those of synthetic examples, but rather several general eastward dipping trends. Which constraints do you apply? Could you provide a plot of these constraints along the 2D section?

Reply: Thanks for noting this, we agree that visualising a constraint like Fig. 2d can be advantageous for the case-study. Not seeing a clear reflector in seismic images in a hard-rock environment is quite common. Also, even if the reflectors were detectible, for assigning different rock units to the reflectors, petrophysical constraint, and other integrated interpretations would be necessary to provide a clear interpretation of the seismic image as what has been shown in the example sections. For the case study section we have done some post-processing on the seismic section to extract some features from the most obvious reflectors so that they could be used for interpretation and extracting constraints. We used Energy envelop of the seismic traces (be it a function of amplitude) to enhance the effects of reflectors within their neighbourhood. Including such a section in the paper requires us to talk about the entire process that was implemented on the seismic section. We believe that people working on seismic datasets can find this way or other alternatives to extract the most detectible features from images easily. We have attached a Figure in this document regarding the section from the seismic image that was used for extracting constraints in the case study section (Fig. 1_2). The original size of the seismic section was (4001*4501) showing the high-resolution image, while for using it as a constraint as explained in the method and introduction sections, it should have the same size as the gravity grid section (20 * 154). Therefore, the interpretations need to be up-scaled and projected onto the gravity inversion mesh. The resulted section is eventually used for further interpretation and constraint extraction. We have used the presented interpretation of seismic datasets in Lindsay et al (2020) to assigned reflectors to different rock units as shown in Fig. 1_2. We prefer not to include the attached section in the manuscript because 1) along with the image we should provide a long section about generating this image 2) the process is mostly related to post-processing technique and is only applicable if the datasets are noisy like what is used in this

study so it might reduce the consistency of the paper and will be beyond the scope of this paper.

We have now added a sentence stating that we use Lindsay interpretations to produce the constraints at lines 448-449.

RC2_18: You mention on line 459 that Goleby et al. (2004) and Lindsay et al. (2020) use different seismic profiles. On line 341 you mention that you use Goleby interpretation. Is your seismic profile coming from the 2004 study or the 2020 study?

Reply: Thank you for this careful remark. After re-reading the text we agree that the original manuscript was confusing. We have made corrections to the text at lines 360-361 and 366-367 to be consistent and stating that we use interpretation from Lindsay et al. 2020. The seismic profile in both studies uses the same data, but Lindsay et al. 2020 reprocessed the data using updated techniques which resulted in slight differences in reflector positioning, signal-to-noise ratio, and detecting the dip of some events. Lindsay et al (2020) use the reprocessed data for interpretation, while Goleby uses the older version. We use the seismic line that has been re-processed later and is utilised by Lindsay et al (2020). The presented result in Lindsay et al (2020) does not very much contradict with Goleby's result. The main difference between the two studies has been pointed at lines 479 to 481.

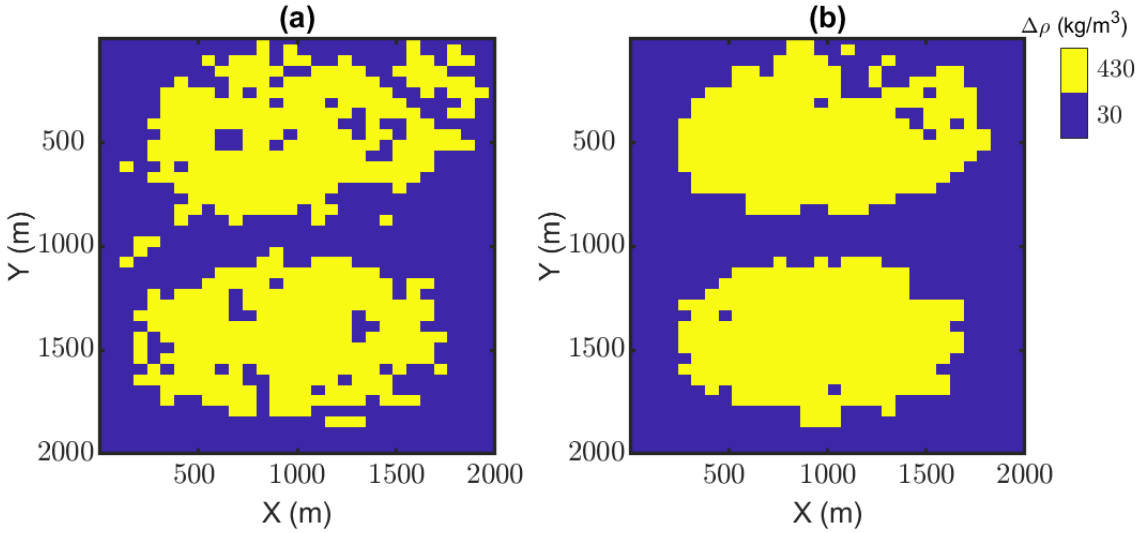

Fig 1_1: Top view of the hard-rock synthetic example at the depth of 150 m. (a) and (b) show the results of the unconstrained inversion without applying the morphological closing to the model and after applying the morphological closing constraint respectively.

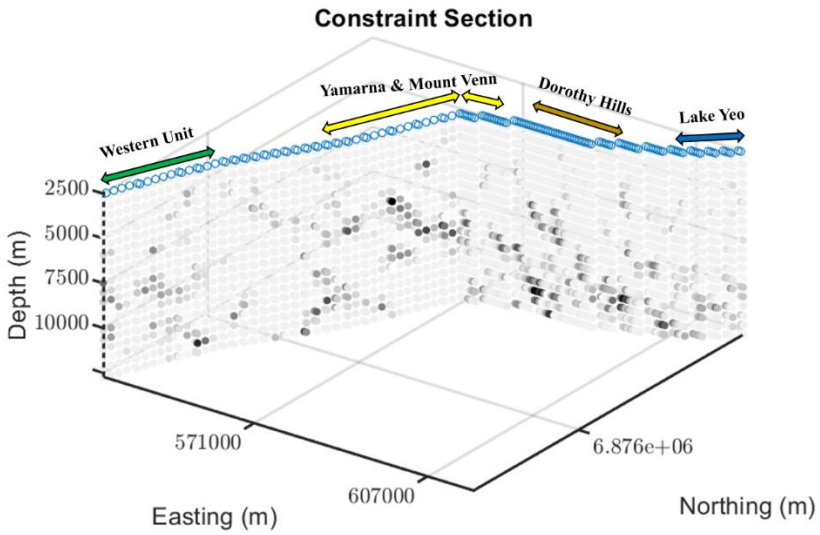

Fig 1_2: Up-scaled extracted seismic reflectors from the original seismic image for the constraining purpose of the level-set inversion in the Yamarna Terrane.