Manuscript: egusphere-2023-129

Object: answer to Anonymous Referee #1, comment posted on 06 Mar 2023

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Dear Reviewer,

Thank you for taking the time to review our submission and for your comments. Below you will find our answers in blue.

We appreciate your positive feedback.

Best regards,

The Authors

After carefully reading and evaluating "Integration of automatic implicit geological modelling in deterministic geophysical inversion", I am impressed with the thoroughness and meticulousness of the research. Good work! The authors have made a substantial contribution to both the geophysics and geology communities with their framework, which can be readily applied to a range of geoscientific problems using gravity data. This includes exploring critical minerals and mapping volcano structures. Overall, I believe this manuscript is of significant importance and quality, and I am pleased to recommend it for publication in Solid Earth, pending a moderate revision.

Thanks for your feedback!

Below please find my major concerns followed by specific comments.

Major concerns:

1. The quality of the geological model is a critical aspect of the framework presented in the manuscript. It is noted that constructing a detailed prior geological model is not commonly practiced, as it requires a significant amount of field geological data and expert knowledge. A reference model that contains incorrect information may guide inversion in the wrong direction, even though the uncertainty may be reduced. The question arises as to whether geophysical data can correct any errors in the reference model. The authors mention that "their approach allows for the inversion to explore a part of the model space that remains within the neighborhood". However, it is unclear how robust this method is. Therefore, further clarification on the efficacy of this approach is warranted, especially in dealing with errors in the reference model.

This is correct. Two aspects can be considered in this question.

The first aspect relates to the impact of poor starting geological models. This has been investigated for the multi-unit geophysical inversion in previous works by Giraud et al. (2021) and Rashidifard et al. (2021), which have shown that, to a certain extent, the type of modelling we propose is robust to errors in the geometry of geological units. RC2 and RC3 raised the issue of using incorrect starting models and we refer to our answer to RC2's first point and RC3's third point for more details. We performed several tests to investigate the impact of a geologically incorrect starting model and found that our method is robust to this to a certain extent (see Figure we added in Section "5.3. Improving the geological realism of a pre-existing model", and "Appendix 4: Robustness to a degenerate starting model with noisy data" and "Appendix 5: Robustness to errors in the density of rock units").

The second aspect relates to conflicts between geological concepts or parameterization and geophysical data. We agree that this calls for further scrutiny. You wrote "The question arises as to whether geophysical data can correct any errors in the reference model." The answer to this question is negative, as some errors that are not incompatible with the geophysical data may persist due to the non-uniqueness of the inverse problem. However, the severity of such errors may be reduced (see the examples we ran with poor starting models). We argue that errors in the geological parameterisation such as the number of rock units or, more importantly, the geological principles that are used, may be deduced. For instance, one may compare the data misfits for the case with geological correction, and without. In the event that the geological parameterisation is affected by such errors, it is likely that the application of a geological correction or using geological prior model term might prevent proper convergence of the inversion.

2. I recommend that the authors provide further elaboration on the term "rock unit" utilized in the manuscript. Although it is mentioned that each unit is associated with a unique range of physical properties and retains constant physical property values during inversion, it is unclear whether a unit corresponds to a single lithology or a mixture of multiple lithologies. Additionally, it is possible for a single lithology to be present in zones that exhibit varying degrees of alteration, mineralization, or mineral assemblages, leading to different physical properties. As a result, further clarifications regarding the definition of rock unit are required to enhance the understanding of the framework presented in the manuscript.

We agree with this comment. What we call a 'unit' is a unit in the petrophysical property contrast sense. Each 'unit is a geological entity that has a petrophysical value (here: density) that is different from the rest. For instance, it is therefore possible for several rock types from the same stratigraphy to fall under the same 'unit' in the modelling approach that we follow.

We clarify this in the methodology section in Section 2.1 by appending the following sentence (underlined text added):

"The method we present relies on the formulation of the model using an implicit model formulation in the form of signed distances to interfaces between rock units. As proposed by Giraud et al. (2021a), this modelling approach considers 'rock units' as one or more rock types characterised by the same physical value (e.g., here, each unit is characterised by a single density value within the modelled area). Each rock unit is modelled by a unique signed-distance scalar field covering the study area. In a study considering n_r rock units of known contrasting physical properties, we consider a set of n_r signed-distance fields $\boldsymbol{\phi} = \{\boldsymbol{\phi}_k, k = 1, \dots, n_r\}$ over n_m model cells corresponding to the distance to the boundaries of rock units."

In the discussion, we added the following in Section 6.2:

"It is therefore possible for several rock types from the same stratigraphy to fall under the same 'unit' in the modelling approach that we follow."

3. Perturbing dipping angle, azimuth, and strike for one or multiple units is a simple way to quantify the uncertainty of the deterministic inversions. Have you done any experimental results regarding uncertainty quantification? I would suggest mentioning UQ in Discussion.

The interpolation algorithm used in LoopStructural minimises the misfit between the constraining data and the regularisation term (smoothing). This means that adding uncorrelated noise to the constraints through a perturbation would introduce a local misfit, the impact of which would be removed, or reduced significantly, by the regularisation. An example for this is presented in Grose et al. (2021) which shows a comparison between radial basis function and discrete interpolation for noisy data points.

Nevertheless, it would be possible to force the perturbed data points to be more strongly weighted in the model to generate different geological models. We argue that perturbing the area in the geological model that is actually constrained by geological observations may not achieve the desired outcome of simulating geological uncertainties. We argue that uncertainties increase away from observations due to the lack of geological knowledge used during interpolation but this is not necessarily captured when perturbing observations. In the scheme of a geophysical inversion, these models might show areas with higher uncertainties around the locations of observations and of structures that are constrained by the geological data and not elsewhere. Ideally, combining geological modelling and geophysical inversions will help geophysics inform the model away from geological data.

We agree that UQ is an important aspect, and it is a topic that we are currently investigating. We are considering perturbations of inversion results to perform null space analysis, but this is not the object of this submission and doing so would make a lengthy paper. Nonetheless,, we have added the following to the discussion (Section 6.1):
"Further considerations of uncertainty may be required to better evaluate and understand inversion results. For instance, the approach of Wei and Sun, 2022, who generate series of inverted models by varying their

deterministic inversions' hyperparameters could be a source of inspiration for uncertainty estimation. Likewise, the scalar field perturbation of Henrion et al., 2010, Clausolles et al. (2023) or Yang et al. (2019) could be transposed to the modelling approach we propose here."

We appended the following to the discussion (Section 6.2):

"Finally, as mentioned in several places in the paper, further considerations on uncertainty are also required to better understand inversion results and find a set of admissible models, both geologically and geophysically."

And also added elements of discussion in Section 6.3 as we detail in our answer to you next point.

4. The assigned density values utilized as a priori information can have a significant impact on the resulting model recovery. Small density values may lead to an overestimation of the rock unit's volume, resulting in a large and less dense body, while large density values may result in the underestimation of the volume corresponding to a small but dense body. To provide a more comprehensive understanding of how prior physical property values affect model reconstruction, it would be valuable to include numerical results reflecting the impact of the assigned density values. This information would enable readers to appreciate the extent of the influence of the a priori information on the inversion outcomes and aid in the interpretation of the model results.

   We agree. Generally speaking we can expect (and have observed) that overestimating the density of a rock unit will lead to underestimating its volume, and conversely for an underestimation of density. In other words, the rock unit affected would either inflate or deflate depending on whether the density is underestimated or overestimated. This is illustrated by additional tests we performed using the first synthetic model. The Figure reproduced below was added as an Appendix to the manuscript.

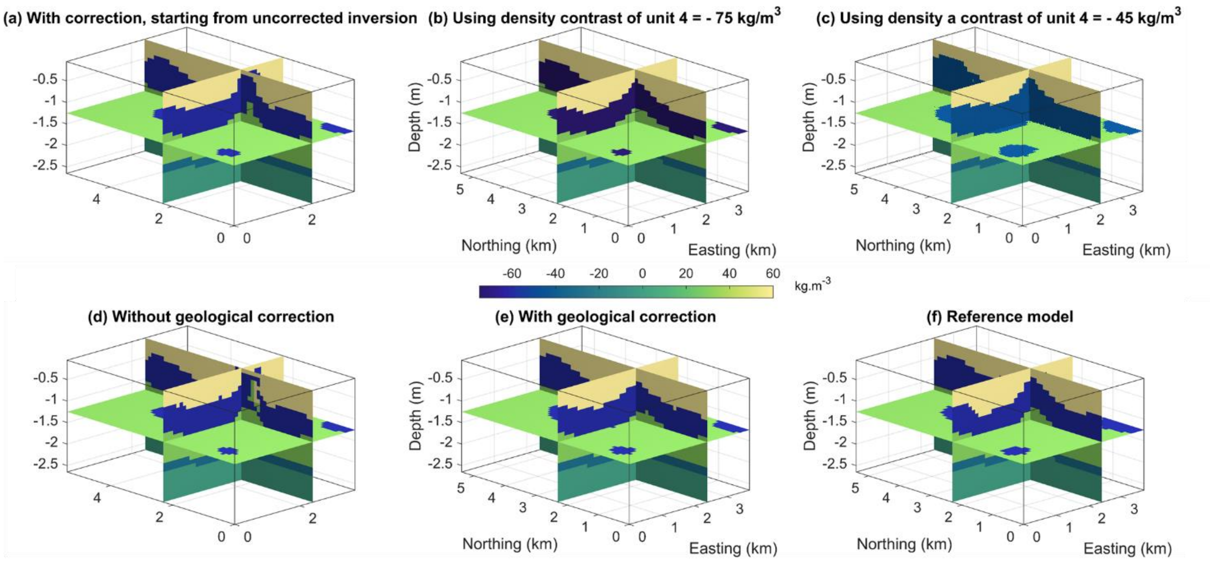

Figure 1. Comparison of inversion results with (a) geological correction starting from inverted model obtained without geological correction, as shown in (d); results with geological correction at each iteration with underestimated density contrast (c), overestimated density contrast (d) for unit 4. The case with accurate density contrast for all units unit and the reference model are show in (d) and (e), respectively.

We have add this Figure in an appendix (Appendix 'Robustness to errors in the density of rock units') along with a paragraph discussing the results.

The importance of prior information such as the number of units or their density has been investigated in a previous work using a similar approach, e.g, Giraud et al. (2021). Nevertheless, we agree that this is important and have added the following text to further discuss the importance of prior models.

We modified the discussion in Section 6.3 as follows (underlined text added):

"~~Last, extensions of our method may allow null-space exploration and to mitigate some of the limitations exposed in the previous subsection~~. Finally, extensions of our method may allow for null-space exploration and the mitigation of some of the limitations identified in the previous subsection. This paper investigates the importance of ~~the prior modelling and~~ geological information in level set inversion. Previous work focusing on level set inversion following an approach similar to ours have investigated the importance of accurate knowledge on the geometry and the number of rock units a priori (Giraud et al., 2021a). Giraud et al., 2021a, and Rashidifard et al., 2021, suggest that inversion is somewhat robust to errors in the starting model geometry and in the petrophysics of the rock units. However, results from Giraud et al., 2021a, using synthetic models suggest that level-set inversion "presents limitations when an important geologic unit is missing from the initial model". To alleviate this, ways to generate the 'birth' of new geological units for inversion to consider geological bodies previously not accounted due to lack of information may be devised. One possibility could be to use the sensitivity of geophysical data to changes in physical property."

Specific comments:

The manuscript is in a good shape, I just have a few minor comments.

Page 2L40: It is recommended that the authors consider citing the work of Wei and Sun (2022) in the manuscript. Wei and Sun quantified the uncertainty of rock units derived from geophysical joint inversion. Including a citation to this work would provide readers with additional context and insights into the understanding of rock units.

Wei, X. and Sun, J., 2022. 3D probabilistic geology differentiation based on airborne geophysics, mixed L p norm joint inversion, and physical property measurements. Geophysics, 87(4), pp.K19-K33.

Thanks for the reference. We have added the following to the discussion (same text the answer to point 3 above about UQ).

Section 6.1:
"Further considerations of uncertainty may be required to better evaluate and understand inversion results. For instance, the approach of Wei and Sun, 2022, who generate series of inverted models by varying their deterministic inversions' hyperparameters could be a source of inspiration for uncertainty estimation. Likewise, the scalar field perturbation of Henrion et al., 2010, Clausolles et al. (2023) or Yang et al. (2019) could be transposed to the modelling approach we propose here."

Section 6.2:
"As mentioned in several places in the paper, further considerations of uncertainty may be required to be able to better understand inversion results."

Section 6.3:

"… constitute a promising area of research for future work, and that uncertainty quantification needs more investigations"

Page 19 Figure 11: I would like to see the observed gravity data in Fig 11 as well, which can tell the mismatch between observed data and simulated data using reference and starting model.

We have added the following underlined text to the manuscript in Section 5.2.1.:

"The gravity data simulated for the reference and starting models are shown in Figure . We consider the data produced by the reference model as the field measurements corresponding to the model we try to recover."

In the caption of Figure 11, we have added the following:

"Figure 11. Gravity data simulated for the reference model (left), which we consider as the field data that invert, and for the starting model (right), which corresponds to the starting point of inversions."

Page 22 Figure 15: It is not clear from the manuscript why Cases 2, 3, and 4 do not converge.

All inversions actually do converge to a stable solution to a similar data misfit of 0.5 mGal. However, they converge to different models, each of which is characterised by a different value for OC, $ERR_{\boldsymbol{m}}$ and ERR_{ϕ}. We have added the following clarification (Section 5.2.2):

"This observation is further confirmed by the metrics shown in Figure 12. All four inversions converge to different models, each of which is characterised by a different value for OC, $ERR_{\boldsymbol{m}}$ and ERR_{ϕ}."

References

Clausolles, N., Collon, P., Irakarama, M., and Caumon, G.: Stochastic velocity modeling for assessment of imaging uncertainty during seismic migration: application to salt bodies, Interpretation, 1–67, https://doi.org/10.1190/int-2022-0071.1, (2023).

Giraud, J., Lindsay, M., and Jessell, M.: Generalization of level-set inversion to an arbitrary number of geologic units in a regularized least-squares framework, GEOPHYSICS, 86, R623–R637, https://doi.org/10.1190/geo2020-0263.1, (2021).

Grose, L., Ailleres, L., Laurent, G., and Jessell, M.: LoopStructural 1.0: time-aware geological modelling, Geosci. Model Dev., 14, 3915–3937, https://doi.org/10.5194/gmd-14-3915-2021, (2021).

Henrion, V., Caumon, G., and Cherpeau, N.: ODSIM: An Object-Distance Simulation Method for Conditioning Complex Natural Structures, Math. Geosci., 42, 911–924, https://doi.org/10.1007/s11004-010-9299-0, (2010).

Rashidifard, M., Giraud, J., Lindsay, M., Jessell, M., and Ogarko, V.: Constraining 3D geometric gravity inversion with a 2D reflection seismic profile using a generalized level set approach: application to the eastern Yilgarn Craton, Solid Earth, 12, 2387–2406, https://doi.org/10.5194/se-12-2387-2021, (2021).

Wei, X. and Sun, J.: 3D probabilistic geology differentiation based on airborne geophysics, mixed Lpnorm joint inversion and physical property measurements, Geophysics, 87, https://doi.org/10.1190/geo2021-0833.1, (2022).

Yang, L., Hyde, D., Grujic, O., Scheidt, C., and Caers, J.: Assessing and visualizing uncertainty of 3D geological surfaces using level sets with stochastic motion, Comput. Geosci., 122, 54–67, https://doi.org/10.1016/j.cageo.2018.10.006, (2019).