

Response to referees, hess-2017-734

Firstly, the authors would like to thank the three anonymous referees for taking their time to read the manuscript and providing detailed and constructive comments. The comments, questions and suggestions are addressed in the following response.

***RC: Referee Comments**

***AC: Author Comments**

Response to anonymous referee #1

General comments:

'The main subject of the article is studying the impact of datasets used to do hydrostratigraphic modeling with the MPS framework. The authors build a "Base Case" using snesim approach, with a cognitive model as Training Image (TI), borehole data as hard data and geophysical resistivity data (SkyTEM) as soft data. Then, they present different modeling cases: using a different TI, using an incomplete resistivity grid instead of a full resistivity grid, using borehole data as soft data instead of hard data, inverting resistivity data with a sharp inversion model instead of a smooth inversion model. The authors assess qualitatively and quantitatively the impact of changing each of these parameters. The main contribution of the article is the method to compare quantitatively the great number of geostatistical realizations (400). The method used is based on Analysis of Distance, with the Euclidean Distance Transform (EDT) algorithm applied to measure the "distances" between realizations. The distances serve as measures of similarity between the different cases and also between cases and the TI. According to the reviewed article, the EDT is straight forward method to assess the dissimilarity between realizations that can help in the quantification of the uncertainty of the 2D and 3D models. The smaller the distance, the more similar the realizations and thus, the smaller the impact of the changed parameter on the modeling results. It is a contribution because not many hydrogeology articles are found on the "metrics" for comparing geostatistical realizations. Plus, distance measures are discussed on MPS literature but for their use in pattern modeling from training images (Gregoire Mariethoz and Caers, 2015; Honarkhan, 2011), not for their use in uncertainty estimation. In the recent book from Mariethoz and Caers (2015), called "Multiple-point geostatistics: stochastic modeling with training images" the use of distance transforms for uncertainty purposes is not mentioned. Furthermore, in the review papers on MPS methodology, the study of the sensitivity of the model prediction to TIs and underlying datasets is suggested as an important research avenue (Hu and Chugunova, 2008).

The paper is well written, with good story-telling. Even though several cases are presented, the structure is logical and the discussion about the results of each case is clear thanks to the images presented. I would agree with the publication of this article because the method seems to be a contribution with the uncertainty appraisal of the MPS results.'

RC1: *'Although the proposition to use distances to assess uncertainties is interesting, it seems to me that the simple EDT is not the most adequate to capture the differences between realizations. To give one example, in figure 9 we can see that the results from "Case 1a" and "Case 1b" are very different (basically, sand to the west and clay to the east for Case 1b while Case 1a is heterogeneous in the whole model). Nevertheless, in figure 11 both cases present the same distance to the cognitive geological model. The qualitative assessment by visual*

means remains necessary. Did you consider using more robust methods for comparing patterns in images which take into account the positioning of the events (spatial relations) and that are less affected by scaling, rotation and translation (e.g. SIFT, IMED)?'

AC1: The usage of the simple EDT for computation of the 'distance' between different realizations is a computationally feasible method for comparing 400 realizations each containing 229*133*39 cells (1,187,823 cells). The EDT method was therefore used because it thoroughly compares the average mismatch between the different realizations. However, we agree that the method is a bit simplistic for comparing heterogeneous geological objects. Other methods were in fact considered, but the EDT-based approach was the most suitable for getting started with research into comparing stochastic MPS modelling. It would be interesting to study, but was left out of the paper to keep focus on the large number of cases and assessment of the uncertainty related to them.

Changes to the manuscript: We will mention that other methods for comparing realizations exist in the introduction on page 5 lines 21-32 and add a few sentences more in the discussion section on distance measures on page 32 lines 5-17.

RC2: *'On the Kasted TI and the conceptual TI we observe channels filled with one facies, without internal variation. How come there are these intercalations of sand and clays in the simulation results?'*

AC2: This is due to the fact that the simulations are probabilistic in nature, and are based on random processes. At the beginning of the simulation a random path is drawn so that the simulation grid is filled by visiting each grid cell only once. The fine-scale patterns are partly due to the hard data which are inserted into the simulation grid before the simulation commences, and is excluded from the simulation path. As the grid is filled out, the hard borehole data might suggest a certain category but the soft data suggests another category. As the grid is filled out the overall category from the soft data dominates and if the random path visits the grid cells near the hard data point towards the end of the random path, then we are left with a small intercolation (e.g. Hansen et al., 2018). The intercolations are also inherent in the simulations without hard data, and is mainly due to process randomness related to how the snesim algorithm draws from a cumulative density function (CDF) (Strebelle, 2002)

Changes to the manuscript: The above comment did not result in any changes to the manuscript.

RC3: *'As mentioned in the discussion, the global target proportions of the units could have been replaced by the vertical proportions. It would have been interesting to see the results of these realizations with the vertical proportions, but I understand that the authors don't have them (time constraints?). What are the statistics of the results? How are those global proportions respected in each case? How the change of the parameters impacts the global target statistics?'*

AC3: The simulations have not been run with the vertical proportions since this would constitute an entire set of cases on its own, and due to the length of the paper and time constraints this was not considered. Additionally, regarding the compilation of the global proportion statistics, again, this would increase the length of the paper and shift the focus away from the main topic which is using distance based similarity measures for comparing a large collection of MPS realizations.

Changes to the manuscript: Due to the general length of the paper, we would like to avoid adding an extra case and expanding the paper to contain the global proportions statistics for each realization, unless the global statistics reveal some significant patterns relevant to the research topic of comparing MPS realizations using a 'distance' measures.

RC4: *'The article relies on other papers for most of the methodology, but still gives some small descriptions. Nevertheless, nothing is presented on the Direct Sampling Method used for filling the gaps on the resistivity grid. This seems to be missing in the methodology. Also, the choice of the Tau value for resistivity and boreholes (2 and 1) is not argued or referenced. Why 2 for resistivity and 1 for boreholes?'*

AC4: We see your points. The choice of Tau model was purely based on a series of tests, which are not mentioned and should be mentioned. Different combinations of Tau values were exhaustively tested, and the chosen values resulted were chosen since they resulted in simulations in which a smooth transition between borehole conditioned areas and non-borehole conditioned areas was seen.

Changes to the manuscript: A presentation on the Direct Sampling Method used for filling the gaps in the resistivity grid will be added as a section in 2 Materials and methods. It will be added to the text that the choice of Tau values are based on exhaustive tests.

RC5: *'What could the authors infer about the impact of the datasets in areas where data is less dense? The study case in Denmark has good data coverage, both for geophysical surveys and for borehole data.'*

AC5: When the dataset is less dense than the Kasted dataset, the simulations have less soft data for conditioning. The less conditioning data which is available, the more the simulation relies on the TI for conditioning. An extreme of this scenario is when no conditioning data is used, and the realization is entirely unconditioned (e.g. Strebelle and Journel, 2000). Therefore, the choice of TI would impact the simulation result in a larger degree if less conditioning data is present.

Changes to the manuscript: A description of the above might be added to the manuscript, provided a logical place is found.

Technical comments:

- It is not indicated what "SkyTEM" stands for.
 - It is a system name for an airborne transient electromagnetic system, which will be mentioned when it is first used in the abstract.
- Page 4: "Two approaches are taken"? ... we are expecting a second approach...
 - Yes, the other common approach should be included in this paragraph.
- Page 7: Realizations THAT reflect the real world
 - P. 7 line 15: this will be corrected in the revised paper.
- Page 15: if the grid is too sparse, then limited or no information is present which can help reconstruct missing patterns is present (repetition of "is present")
 - P. 15 line 9: this will be corrected in the revised paper.
- Page 29: "increased"

- P. 29 line 18: this will be corrected in the revised paper.
- Page 21: comparing a “realization” (no “s”)
 - P. 21 line 26: this will be corrected in the revised paper.
- Page 35: Journal, A. G.: "Combining Knowledge From Diverse Sources: An Alternative to Traditional Data, , 34(5), 2002". (The name of the Journal is missing, “Mathematical Geology”)
 - The mentioned reference will correctly contain the journal name in the revised paper.

Response to anonymous referee #2

General comments:

'The manuscript "Contributions to uncertainty related to hydrostratigraphic modeling using Multiple-Point Statistics" presents an interesting study where the uncertainty related to the input data required by a multiple-point statistics (MPS) simulation framework is investigated. The research described in the manuscript, although focused on a specific case study in Denmark, could have a broader applicability and would probably be of interest for the HESS readers.

Nevertheless, I believe that the manuscript contains some major issues that should be addressed by the authors before its publication. In particular, my concerns are related to three aspects: 1) The structure of the manuscript, 2) some missing details/discussion about important aspects of the parameterization of the methodology, 3) the way mathematical relationships are expressed.'

RC1: *'Manuscript structure: A number of techniques are used within the manuscript to complete the quite complex simulation framework. Some of them are used multiple times and in different contexts (for example, the tau model). Therefore, putting their description in a separate section "Methods" would be much more helpful and would help the reader in orienting himself inside a quite complex work-flow. At the moment, the description of the methods is spreader all around the manuscript, sometimes together with the results, quite often with some repetition, which makes reading the manuscript not a smooth task. A clear example of this "breaking the rhythm" of the manuscript is for example at page 18. Also, here the description of the technique is made at the wrong place, because the method was already applied some step before in the work-flow. Another example is at page 21, where a 2D example is introduced to explain the EDT.*

In addition, the comparison methods (EMR-maps,...) and the distances (EDT...) definitions would deserve a separate section, maybe just after or within the "methods" section. There are also many locations, in particular in the "Results" sections, where too many details which would be more appropriate for the "Discussion" section are anticipated (see for example pages 27-28, lines 6, 10-11).'

AC1: Under the preparation of the manuscript we have worked iteratively on the structure of the manuscript and ended up with this structure as the most reader friendly consisting of a large Material and methods section (section 2), divided into the study area (2.1 The kasted study area), a general method description section (2.2 Multiple-Point Statistics (MPS) and single normal equation simulation (snesim)), a detailed description of the MPS modeling set-up with the methods related to each case (2.3 MPS modeling setup) and lastly a section of the methods used for comparing the simulation results. Generally, the style chosen for this manuscript was to explain some of the methods utilized in the, as mentioned, quite complex simulation framework was to use practical examples. This often aids the reader with figures and a purpose for applying the given method.

For instance, the usage of the Tau model is used in different contexts and is clearly explained in section "2.3.5 Case 4 – borehole lithology logs". It therefore seems unwarranted to create a separate section, which repeats the entire description of the Tau model. Alternatively, the detailed description of the Tau model could be removed from section "2.3.5 Case 4 – borehole lithology logs", but the authors prefer to present the Tau model with a specific case in mind. In this scenario we used case 4 to describe the usage of the Tau model, since the reader would be able to use Figure 7 as a visual aid in understanding the Tau method.

Changes to the manuscript: The method descriptions which are not found in section "2 Materials and Methods", but instead are found in section "3 Results", as mentioned by Anonymous referee #2, should be moved to section "2 Materials and Methods". However, brief descriptions which are used to help the reader,

e.g. P. 23 lines 14-15 where the EMR maps are briefly explained again, should not be moved to section "2 Materials and Methods".

RC2: *'Section "Basic modeling set-up": This section is somehow quite confusing, because the authors mix the description of the "Basic modeling set-up" with the Egebjerg TI description. I suggest to better separate the description of the various cases.'*

AC2: This was a mistake. The reference to Table 2 for some reason included text from the section above or below Table 2.

Changes to the manuscript: The Egebjerg TI description will solely be placed in section 2.32 Case 1 – Conceptual geological understanding.

RC3: *'Tau model usage: The tau model represents one of the crucial steps of the methodology, because it is used to take into account the soft constraints provided by geophysics, but also to combine the "borehole probability" with the SkyTEM one (Fig.7). Although some information about the tau weights are provided (i.e., in appendix), I would suggest to discuss at least briefly their choice. For example, many of the considerations made by the authors would be strongly influenced by the choice of the tau weights (see for example line 32, page 30). Some insights about the choice of these weights are provided by Allard et al (2012, DOI: 10.1007/s11004-012-9396-3). Also, what happens when the weights are_1? (see pp18, equation 2).'*

AC3: Here we refer to the Author Comment 4 (AC4) in the response to anonymous referee #1. Briefly, in relation to the choice of Tau parameters for the Tau model it should be mentioned that a series of tests have actually been carried out to select the final Tau values.

Changes to the manuscript: It will be added to the text that the choice of Tau values are based on exhaustive tests.

RC4: *'Case studies labelling: The provided table that summarizes all the case studies is of course useful, but overall into the manuscript (for example, in figure captions), there is very often a redundancy and some of the details of the different methods, which are repeated multiple times. Maybe you should reference much more often to Table 1 and to the "codes" like "Case 1a", "Case 1b" only, and avoid repeating the detailed differences. One example of these repetition can be observed in Figure captions (see for example Fig.9, page 25).'*

AC4: This would certainly make the paper more concise in certain parts. However, it would also require the reader to constantly avert his/her attention to Table 1.

Changes to the manuscript: In the revision of the manuscript Table 1 will be referenced more often to avoid repetition, to the extent we find reasonable without disturbing the reading experience.

RC5: *'Introduction pp4, lines 20-XX: Here I would also mention the problems related to the solution of the inverse problem (IP) in itself. By the way, this also somehow motivates your efforts in trying two different inversion techniques, like SCI and sSCI.'*

AC5: This is a good point.

Changes to the manuscript: A brief description of the problems related to the inversion process will be added to the introduction.

RC6: *'pp5, lines 27-: Here I believe you are already providing too much details for an introduction.'*

AC6: Okay

Changes to the manuscript: we will try to provide less details in the Introduction in the revised paper.

RC7: *'Mathematical formulation: The mathematical formulation is often cumbersome, because very often long text lines are used to define quantities and as subscripts. I strongly suggest to lighten the notation avoiding long text lines, and using the many letters provided by the alphabets. For example, N and M could be used instead of Nrealizations and Ncells; another example is the definition of $D_{i,j}$ (page 22). In addition, some relationship could be condensed and generalized. In this way, they could be written only once and contribute to shorten the manuscript. See for example (7) and (8) at page 21.'*

AC7: We agree that the mathematical formulations could be written in a more concise manner. However, regarding eq. (7) and (8), again, we believe it aids the reader to first see the formula with a specific case in mind and then generalize afterwards.

Changes to the manuscript: The mathematical formulas will generally be shortened and simplified for the revised paper.

RC8: *'TI non-stationarity: In section 3.1 but also in other parts of the manuscript the imprecision of MPS in reproducing some features is clearly depicted. However, I believe that many of the encountered problems are due to the non-stationarity of the used TI. Therefore, although of course taking into account for the geophysics helps, I would suggest to at least mention and briefly describe the role of the non-stationarity of the TIs.'*

AC8: The geophysical data is so spatially dense that TI non-stationarity is not as big of an issue as when less conditioning data is present. We therefore decided to not include this complication, to not confuse the reader. However, it might be wise to mention that this is the case and that even though the TIs are non-stationary, the spatially dense geophysical data actually helps in the matter.

Changes to the manuscript: Where appropriate, we will add sentences on non-stationarity of the TIs'.

RC9: *'Variograms: Could you briefly mention which variogram model you used for example to create the borehole footprint (pp18, lines 3-6)?'*

AC9: It is mentioned both in the text where you indicated, but also in the Appendix under section "A1".

Changes to the manuscript: We will add the variogram model type, e.g. exponential, spherical, etc., to the Appendix under section "A1".

RC10: *'Fig.4: Please add a comment related to the spatial scale of the Egebjerg TI, which is quite different from the other two. Also, it would be quite nice to add a sub-figure containing the same vertical proportions for the borehole logs.'*

AC10: That is a good point!

Changes to the manuscript: A comment will be made regarding the fact that the 'vertical scale of the Egebjerg model is quite different from the other Tis. Provided the creation of a sub-figure containing the borehole vertical proportions is not too time consuming, we will implement this sub-figure.

RC11: *'Fig.11: The label "Realization number" in the vertical axis of part A is too close to part B and is therefore misleading. Also, I believe that the results of part B could be condensed using box-plots, one box-plot for each case. In this way, the fictitious and misleading order of the "realization number" would be by-passed.'*

AC11: Yes, the Fig.11B of the figure will be given a bit more space so that it is clear that the "Realization number" is part of Fig.11A. We would prefer to not use boxplots since they mainly provide summary statistics and we would prefer that the reader can see the actual distance values instead.

Technical comments:

- pp6, line 9: Please check the order in "33 line km spatially..."
 - This will be re-ordered correctly.
- pp8, line 30: It looks like the reference to Fig.4 is missing between Fig.3 and Fig.5.
 - We will add a sentence with reference to Fig. 4, so it will be mentioned before Fig. 5
- pp9, line 5: "data is" => "data are"
 - This will be corrected in the revised paper.
- pp18, line 18: "[2,1]" is somehow confusing with the index that you introduce some equations before... I would specify that they are float values, writing explicitly 2.0 or 1.0.
 - This will be added to the revised manuscript.
- pp20, line 25: Maybe "(3)" => "(4)"?
 - This will be corrected.
- pp21, equation (6): Please check for the missing i subscript to v
 - There is no missing subscript. The "u" symbol represents a single location vector, while the "v" is a set of vectors contained by "V". Therefore, the formula only shows the computation of the d_{EDT} at a single location. The process must be repeated for all points for the grid. Perhaps this should be mentioned in the revised paper.
- pp21, line 20: Here Delta appears in the formula, but not in the following text... please check.
 - This will be corrected in the revised paper.

- pp22, line17: "realizations using" => "realizations computed using" (?)
 - This will be corrected in the revised paper.
- pp27, lines 6-11, 30-31: This is somehow repetitive. Please try to avoid repetitions also in other locations in the text, but in particular in this section.
 - We couldn't find the particular repetition mentioned here, but will try to remove as many of such repetitions in the revised paper.
- pp30, line 26: "to alter...?"
 - Will be corrected, however, it seems like it is a logical statement.

Response to anonymous referee #3

General comments:

'This paper is the product of a nice piece of work and is very interesting. My main concerns are related to the introduction, where some transitions and justifications are missing and to the methodological section, that goes too fast into details. I therefore suggest the following minor revisions.'

RC1: *'In the introduction, transitions are often missing between paragraphs, for instance, page 2, between lines 14 and 15. It is a bit jumps from one topic to another. Related to the paragraph comprised between lines 3 and 14, you might cite the following paper that discuss uncertainty and bias in training images : Ferré, Ty. "Revisiting the Relationship Between Data, Models, and Decision-Making." Groundwater 55, no. 5 (2017): 604-614. Pirot, Guillaume. "Using training images to build model ensembles with structural variability." Groundwater 55, no. 5 (2017): 656-659.'*

AC1: Good points.

Changes to the manuscript: The introduction will be cleaned up so that transitions between paragraphs are less abrupt in the revised paper. The two references will also be added in the revised paper.

RC2: *'General justifications are given in the first paragraph of the introduction, but the authors should also justify why they chose this specific sites, and what they bring or want to improve, with regards to previous studies conducted at the Kasted site.'*

AC2: That is a good point. The main justification for using the Kasted site was that the geology of the area was fairly simple, thus the dataset is also, to a degree, simple. Furthermore, a geological model of the area had already been compiled, meaning we already had information about the hydrogeology.

Changes to the manuscript: The justification for using the Kasted dataset should be mentioned in the introduction and will be added. We will also revise the paper so that it reflects what we hope to improve in regards to the Kasted model.

RC3: *'You should also define your notions of hard and soft conditioning clearly in the introduction'*

AC3: Okay.

Changes to the manuscript: We will add this definition in the revised paper.

RC4: *'Then, in section 2, when presenting the study area, the historic of previous research could be explained/clarified. Page 6, line 5: one 'complex' too much? Page 6, line 14: how is defined the 'selected quality threshold?'. '*

AC4: If anonymous referee #3 is referring to the fact that we should explain previous research in the Kasted area, then the main research which has been conducted in the area is compiling the cognitive 3D geological model of the area. Therefore, we do not desire going into more detail.

Changes to the manuscript: The poor usage of the word 'complex' will be corrected. A reference to the borehole quality assessment method used will be added here and the method is briefly introduced.

RC5: *'The main aspect, regarding the method subsection is that the reader is lost in details from the beginning. A big picture of the approach is missing. In the way of presenting, I would recommend to give first an overview of the method, and progressively go into details.'*

AC5: Perhaps it would be wise to include an overview of what we hope to achieve by stochastic modelling.

RC6: *'Page 7, lines 7 to 15 are not very clear. Can you reformulate?'*

AC6: Will be reformulated in the revised paper.

RC7: *'Page 8, line 26, figure 5 is called, while figure 4 has not been called.'*

AC7: We will fix this by adding a reference to Figure 4 before we call Figure 5.

References

- Hansen, T.M., Vu, L.T., Mosegaard, K., Cordua, K.S., 2018. Multiple point statistical simulation using uncertain (soft) conditional data. *Comput. Geosci.* 114, 1–10. <https://doi.org/10.1016/j.cageo.2018.01.017>
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- Strebelle, S.: Conditional Simulation of Complex Geological Structures Using Multiple-Point Statistics, *Math. Geol.*, 34(1), 1–21, doi:10.1023/A:1014009426274, 2002.