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Interactive comment on "3D multiple point geostatistical simulation of joint subsurface redox and geological architectures" *by* Rasmus Bødker Madsen et al.

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We would like to thank Donald Keefer for his referee comments. In the following, citations from the interactive comment are written with RC1 in front of them. From reading the comments, we have not been able to describe and state the work frame and purpose of the project thoroughly. We think that a lot of the comments are based on a misconception of the modeling purpose and detail. Before commenting, we therefore start by stating the purpose of the modeling.

The work we present is part of a project (The Mapfield project) that aims at developing a concept for targeted N regulation. This concept should be consistent with various

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data sources available but should also be cost-effective such that it might be suited for commercial use afterwards. The evaluation of nitrate vulnerability should be based on a standardized workflow and should still be able to be customized to the regional challenges in specific areas.

The modeling purpose of the current study is to create subsurface 3D models of geological architecture and redox architecture to be used in hydrological modelling. Via particle tracking, the reduction capacity for the subsurface can be assessed taking some of the 3D architectural heterogeneities into account. The modeling scale is partly determined by the overall purpose of the project and partly by the typical resolution of EM data. We are fully aware that it is not a perfect description of the subsurface, but reasonable within the scale of investigation. An obvious advantage of using MPS is that the realizations are consistent with the information and inputs selected. If there is some variability that is not geologically correct in the realizations it is not necessarily an issue of MPS modeling but means that this variability is not present in the training data or conditional data. Irrespective of this, we still claim that it is better to integrate this information than not to.

This work is an important step towards solving the aim of the Mapfield project. Additionally, this work is not only of importance in the specific problem of targeted N regulations, but any water quality issues under heterogeneous settings.

Generally, we have clearly not been able to transfer this message in the manuscript and apologize for this. We will work on improving the introduction to the modeling and our justification for using MPS specifically to model spatial patterns in the subsurface.

RC1: "This manuscript is included for consideration of a special issue: Frontiers in the application of Bayesian approaches in water quality modeling. It is important to note that the research described in this manuscript does not use Bayesian methods, and so does not directly relate to the topic of the special issue. "

The manuscript is not considered for the special issue anymore.

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RC1: "Leaching of agriculturally-applied nitrogen is a significant threat to global groundwater resources. Success in reducing nitrate contamination in groundwaters by modification of farming practices and reductions in fertilizer input has been only occasionally realized and more work is definitely needed. Prediction of the fate and transport of fertilizer-based nitrate is a complicated problem that is confounding successful remediations to the groundwater contamination problem. Modeling success is significantly limited by the natural heterogeneities and complexities of the subsurface geologic systems and by our limitations in characterizing and modeling those complexities. The complex nature of the heterogeneities has led to the treatment of these systems as stochastic which has subsequently led to a large interest in probabilistic modeling approaches."

We completely agree with the reviewer that not only is pollution of groundwater resources from surface leaching a significant problem but also that this is a complex problem to solve/model. Especially, given heterogeneities in the subsurface. Regarding the last line. Do you mean that these systems are modeled stochastically in our case specifically or in general? To our knowledge most studies focusing on mapping heterogeneities in geology and redox conditions are not treated stochastically. If you have knowledge of references where redox conditions and geology as a combined system are treated stochastically, we would be glad to know.

RC1: "Multiple Point Statistics (MPS) has proven to be an innovative and successful probabilistic approach to modeling inter-facies relationships, primarily within distinct, lithostratigraphic units. As typically used, MPS is not a method that can be used with stratigraphic units or with units that are genetically distinct (e.g., from subglacial environments and glaciofluvial environments), unless each genetically-distinct succession is modeled within separate portions of the model domain. To my knowledge, a modified MPS approach has not been successfully applied to modeling of larger stratigraphic assemblages of rocks or sediments. It would be particularly relevant and innovative if the authors were to present a method for adapting MPS to stratigraphic unit modeling.

They do not suggest they are doing that here. "

We would like to argue that MPS has not only been successfully applied to model inter-facies relationships. Since the inception of MPS the key feature of the method is the ability to model spatial continuity over longer distances. Mariethoz and Caers (2015) describe their comprehensive book on the application of MPS as: “This book is therefore a book about spatial and spatiotemporal modeling in the physical sciences (sedimentology, mineralogy, climate, environment, etc.)”. In other words, MPS is not scale or problem dependent. Tahmasebi (2018) also showcase different applications of MPS in his state-of-the-art review of the method. Several studies have shown the applicability of MPS for modeling the geological architecture of major lithological units (Jørgensen et al. 2015; Barfod et al. 2018; Vilhelmsen et al. 2019), although we agree that the application of MPS for real world scenarios is not overwhelming. Høyer et al. (2017) are simulating the architecture of a thick succession of Miocene sand and clay units within a confined area of the subsurface. In accordance with this approach the geological elements in the current study confines a volume in which a TI represent the different deposition histories and the expected differences in spatial variability.. Instead of simulating merely sand and clay, in the current study we use 5 lithological groups thereby extending the concept proposed in Høyer et al. (2017). The reason we choose major lithological groups to model in the current work is based on the vertical resolution of both geophysical data and well data. The data does not allow simulation on the scale within lithostratigraphic units. There are several aspects to this.

1) the current discretization of the simulation grid (25m x 25m x 2m) is not able to accommodate internal sediment structures in the specific lithostratigraphic units.

2) It would require an additional MPS simulation step – a sequential process – where the results would predominantly rely on a TI and perhaps a few wells that contain information about grainsize in the lithological description to enable a distinction between fine-grained and coarse-grained material.

3) a more detailed grid than 25m x 25m x 2m would make it difficult to handle subsequent flow and transport modelling and would ultimately have to be re-gridded to coarser grid to a grid approximating the current. The current grid was chosen in collaboration with a hydrologist to determine the smallest discretization that would still allow computationally feasible hydrological modeling at catchment scale

4) We have doubts that this extra complexity of the problem of adding internal structures would have a significant impact on flow and transport models.

RC1: "The authors have done a great job in selecting a globally-significant problem to study. They are also commended for their innovation in wanting to pair joint modeling of geology and redox conditions through MPS methods. In terms of formal review criteria, the scientific significance of this manuscript is 'good' to 'excellent'. The overall presentation is inconsistent, making the presentation quality 'fair'. Some parts are well written and logically argued, but there several important places in the text need more clarity or better explanations. There are a few key places where critical description of methods are missing. "

We very much appreciate the overall positive feedback on our choice of subject and our presentation of the problem at hand. We fully agree that there is an urgent need for methods to enable N-targeted regulations for protection of groundwater resources in countries with extensive agriculture. We intend to review the manuscript carefully for places in lack of clarity and look at places that might need clarification on method. We encourage the reviewer to participate in this process.

RC1: "The graphics are of good quality and well chosen. However, given the small size and high complexity of the models, the color differences in the geologic models are difficult to interpret. The captions often need to be improved; they need clearer descriptions of what is actually shown in each figure. "

Thank you. We will work on improving the colormap and captions of the figures.

RC1: "Importantly, however, I have significant concerns about the scientific quality of key aspects of the study design. Specifically, decisions about the representation of the geology, application of the geologic representation to the MPS modeling approach, and the discussion of the modeling results are all 'fair' to 'poor'. These scientific quality issues are addressed in detail, below. Overall, I believe this manuscript requires significant revisions prior to publication, but that if these concerns are addressed, it clearly merits another review opportunity. The primary problem I see with the scientific quality in this manuscript is that the geologic deposits are represented as simply a succession of distinct textures (i.e., facies), when the depositional origin, size, distribution, and description, suggest the deposits being modeled are a succession of stratigraphic units, with similar textures, that were deposited through an unspecified number of distinct ice events. "

We refer to our modeling purpose stated in the beginning and our responses above.

RC1: "MPS would be a clearly suitable approach if the authors were modeling textural distributions within the meltwater sand/gravel and clay/silt assemblages, or modeling the distribution of textural facies or inclusions of sorted sediments within the till deposits. However, in that situation, they would have to model the main deposit boundaries separately (using some other approach) and later insert the textural simulation results into each main deposit. Instead, the authors are trying to apply MPS to a collection of sediments from two or three distinct depositional environments (i.e., subglacial, proglacial fluvial, and maybe proglacial lacustrine), and from 2-4 distinct ice events. "

We recognize the issue described. Rarely, however is data collected or analyzes made (e.g., grain analyzes) that would provide sufficient knowledge for such a detailed mapping. Especially not at the scale of the catchment area presented. We have therefore decided to split the area into larger geological elements that consists of multiple depositional events. We also refer back to our previous comment on the data resolution.

If there are some geological rules that would fit better with the modeling area the whole idea is that this information can be quantified and added to the model. It would also be possible to combine the current realizations with these explicit rules/information as a sort of inverse problem. Other options include coming up with extra probability grids that could help guide the results. The question is where to obtain the information for these. It is beyond the scope of the current paper but is worth exploring in future studies. We hope that Donald Keefer and others appreciate that this work is a step towards better and more consistent models that integrate information from several sources.

RC1: "This is more than just a conceptual problem. The MPS algorithms use the training image to guide the location of textures, but every texture has a non-zero probability of occurring anywhere in the model domain. This is not problematic when the facies are all generated within one, single depositional environment. It is problematic when the facies are from multiple depositional environments (and from multiple ice events). "

MPS uses training images as analogs of the spatial variability to generate realizations of possible models of the subsurface. The conditional data (wells, geophysics) guide the location of the architecture. Once again, we have probably not been clear enough in delivering the modeling aim and the chosen method. This is unfortunate.

RC1: "Operationally, this matters because under this latter scenario, the realizations can be expected to have sediments from depositional environments and ice events that are randomly out of sequence. Post-glacial sediments can be expected in many subsurface locations. Too much meltwater sediment should be expected within the upper clay till unit. Too much clay and sandy tills would be modeled within the meltwater succession. Since till units are typically associated with distinct ice events, the clay till will be modeled in too many (and maybe occasionally too few) sedimentologic positions to be consistent with the geologic history. "

The current modeling is focused on the architecture of lithology and hence does not account for geological history in the sense of multiple ice events and depositional events. The geological history and processes need to be conveyed (quantified) through the training image. In our case the subdivision of the simulation grid into geological elements also provide a way of conveying geological knowledge into the system. This modeling is not the conclusive description of the subsurface but fits the purpose of the modeling. The hard and soft data available will help guide the sand and moraine clay layers with realistic distributions in the realizations.

RC1: "This also means that your geologic framework will lead to parameterized groundwater models with predictably-incorrect patterns of hydraulic heterogeneity – one of the main things MPS is trying to avoid. "

In which sense is MPS trying to avoid incorrect patterns of hydraulic heterogeneity? The realizations are consistent with the patterns provided in the training image. Then the problem is rather whether the training image is conveying the expected kind of information about the spatial variability. MPS is not trying to do anything except it helps solve the problem of lacking connectivity of features encountered in classical 2-point statistics.

RC1: "While the distributions of units in the valley-fill (Northern buried valley) setting are a bit more complex, for the same reasons this setting appears to be better described as a succession of stratigraphic units. As with the upland succession, modeling subglacial and proglacial deposits as facies within a single zone is particularly problematic with MPS. In a complex valley fill succession that is composed of multiple erosional/depositional events, it can be very difficult to see the resulting biases – you are expecting complex assemblages and complex assemblages is what you get. The logic of the model doesn't change, however, and the errors for the upland will inevitably be carried over to the valley deposits. "

The delineation of geological elements is carried out being fully aware that each element can compose layer successions from several depositional events. Cognitive interpretation and modelling of specific stratigraphical units it not feasible or to strive for within the project frame, instead our key line out is to: a) Interpret independent and important geological elements/successions with each study area, b) within each element 3D training images are set up with the purpose of representing the geological trends of the structural architecture.

We argue that MPS can be used as an important tool in the context of applying dense EM datasets, where the geological elements and the training images are valuable input to guide the realizations of subsurface structures characterized by the main site-specific lithology classes.

RC1: "I noted early in my comments that the presentation quality of this manuscript is not ideal. It is possible that I have misunderstood the geologic setting and the approach taken to configure the MPS in this study. However, the description of the geologic deposits does not provide enough clarity to understand the geologic history of the model domain, or the consequent distribution of stratigraphic units and sediment textures. The authors also do not acknowledge this important geologic constraint to the successful application of MPS, nor do they provide discussions on their rationale for using MPS in this setting or on the design targets for texture proportion and zonation. This prevents a clear understanding of what the geologic history is known to be, and how this modeling approach is being used to reliably model the sediment while using that knowledge as a necessary constraint. "

Here is probably the crux of our disagreement. As mentioned earlier, we have simply not been able to convey our modeling objectives clearly throughout the manuscript. We do not seek to provide a full description of the geological history of the area. This is not the aim of the paper. Our scientific contribution is to jointly simulate and determine the distribution of redox, geology (here lithological groups). We agree that our presentation of the geological modeling choices have not been sufficient and that we should provide more justification for the way the training images have been constructed. Herein lies most of the geological modeling choices.

RC1: "My last comment regarding the poor scientific quality addresses the poor quality of simulation results for the geologic deposits. Based on the figures of the model realizations and from one or two oblique comments from the authors, these results appear to have an unacceptable fit with the data and training images. The authors barely note the quality of fit in their discussion and (except for a reference to unspecified algorithmic artifacts that generate occasional small errors) they do not provide sufficient technical explanation of why the simulation results fit so poorly with the geology training images. "

We are not quite sure what is meant here? MPS precisely creates a "fit with the data and training images". It is supposed to create conditional simulation based on the training images and the selected parameterization (prior information). Realization are forced to abide the conditional data which ensures that models are consistent with both data and prior information.

RC1: "More importantly, the authors suggest that they could have made the solutions better fit the training images, but stopped with the simulations so they could present the method as a viable option. This needs to be fixed prior to submitting a methods manuscript for publication. Until an author can demonstrate clearly and objectively that they can reliably meet the stated modeling goals using the proposed method, the method is not ready for publication. Acknowledging these limitations within the manuscript, the authors are encouraged to fix these issues, remodel the area, and revise the manuscript. If these issues are corrected, this manuscript would be a worthwhile contribution to the literature. "

The solutions (realizations) are not supposed to fit the training image. Conditional simulation (of any geostatistical simulation methods) generates realizations consistent with the assumed geostatistical model (here in form of the TI and choice of simulation algorithm) and the conditional data. Apparent 'artifacts' simply illustrate that (over longer distances) it is difficult to integrate the two types of information, as they provide different types of information. We have also adapted postprocessing procedures to remedy most of these artifacts.

This is less of a problem using 2-point based Gaussian simulation, in which one will have less of these ‘inconsistencies’ due to the high entropy of a Gaussian model. In general, MPS is based on a limited sized training image and based on higher entropy models. This combination suggests that, in general, one rarely have perfect consistency between the training image and the conditional data. (the conditional data does not appear as is in the training image). This should be noted, as we do in the text, but we do not think an analysis of this challenge should be part of the present manuscript but would warrant a separate independent work.

The solution should be consistent with the data, which is the case. We can try to come up with a way to quantify this statement to demonstrate it more objectively. We specifically wrote the following: “As pointed out by Tahmasebi (2018), a quantitative evaluation of the performance of MPS is still unresolved, and as previously mentioned, the parameterization could potentially be fine-tuned to produce even better results.” What is meant here is that different parameterization of the problem provides different solutions (different variability given the same training image) and it is still difficult to find a universal measure for determining whether the current parameterization provides a better fit or not. We have chosen to avoid this discussion in detail since it could easily become a paper on its own as there is much to explore once you open this discussion. The topic of choosing a suitable parameterization of the sampling algorithm has drawn increased attention in the MPS community within the last years. Exemplified e.g., by the new study by Juda et al. (2020). Basically, there are three main targets for an algorithm parameterization. 1) Realizations should fit the data as good as possible 2) The realizations should convey the underlying patterns and structures in the training image and 3) The realizations should be feasible to compute. This is usually a trade-off situation. Here we focused primarily on making sure that realizations are consistent with our expectation of the variability: “However, we adapt the heuristic strategy of Høyer et al., (2017), making sure that the realizations are in accordance with our expectations and focus on presenting the methodology of simulating both geology and redox simultaneously in 3D high-resolution.”

Kind Regards

Rasmus and co-authors

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