Hydrol. Earth Syst. Sci. Discuss.,
https://doi.org/10.5194/hess-2020-444-AC2, 2020

Hydrology and Earth System Sciences
Open Access
Discussions

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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Received and published: 5 November 2020

We would like to thank the anonymous reviewer for his/her referee comments. In the following citations from the interactive comment is written with RC2 in front of them.

RC2: "Overview: This paper presents an approach for joint stochastic simulation of subsurface geological and redox architectures in 3D using multiple point geostatistics (MPS). The method is demonstrated on a small catchment in Denmark, where simulations are conditioned on observed resistivities of the subsurface from towed transient electromagnetic measurements (tTEM) as well as on soil maps and borehole observations of lithology, sediment colours and water chemistry. The paper is interesting

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and addresses an important topic which fits the scope of HESS. To predict the transport and fate of nitrate and to improve the understanding and management of nitrate contaminated aquifers, detailed knowledge of subsurface geology and redox conditions is required. The characterisation of the subsurface is usually largely based on borehole data (sometimes together with other ancillary data, knowledge etc.), which subsequently are interpolated to cover the domain of interest. The heterogeneity of the subsurface means that such interpolations can be associated with large uncertainty. Stochastic geostatistical approaches, like the one used by the authors here, are therefore widely used to account for such uncertainties in subsurface mapping and modelling. I'm no expert in MPS or geologist (this is therefore likely to be reflected in my comments below), but to me, it seems appropriate to use the MPS method for the context here, although other methods exist. There is therefore a lot to like about this paper. However, I have number comments and issues that I think should be addressed before this paper can be published. Below are my comments which I hope the authors will find useful. Held og lykke!"

Thank you ("mange tak") for the fine review of the manuscript and the modeling objectives. We have found all the general comments provided much useful and will be answered in the following. We will specify what changes this bring about in the coming version of the manuscript.

RC2: "General comments: 1. I'm not very familiar with the MPS method and how it works exactly, so I can't really comment on the chosen parametrisation or even on whether the results produced are good/acceptable. However, I do wonder why the simulation artifacts occur? I think this should be elaborated on. It is stated that the geological artifacts are likely due to inconsistencies between TI and conditioning data (L565), but what does that mean exactly?"

The main idea behind MPS is that spatial variability is described through a training image. For most MPS algorithms a realization is generated sequentially one voxel at a time. Consider standing at some location in the simulation grid and wanting to know what value to realize in this position. You then gather configuration of the surrounding already simulated nodes (conditional event). Specifically, in direct sampling, as used here, you then search the training image for a matching event. If such an event exist it is placed in the simulation grid and you can move to the next location and so forth until the entire simulation domain is filled.

Artifacts in the simulations might occur if it difficult to find a matching event in the TI. This is what is meant by line 565. If at some point it is impossible to find a suitable candidate, the next best thing must be selected. Sometimes this process leads to simulation artifacts. There are several ways this might be remedied but it all comes at a price. In all cases you are trying to broaden the number of possible matches in the training image (i.e., making sure the prior information is not in opposition to the conditioning data)

A simple way is to reduce the number of already simulated nodes to include in the conditional events. With smaller conditional events, more locations in the TI will be considered reasonable matches. This affects the ability to correctly represent the variability in the long-range structures from the TI. In general, it will lead to increased variability that is not necessarily related to geological variability as portrayed in the TI. Also, when simulating using fewer conditional data, the point being simulated might end up leading to inconsistencies for points to be simulated later.

These problems do not arise in 2-point based Gaussian simulation, because one can always compute the conditional distribution, while in MPS one must infer the conditional from a finite sized example (the TI) represent an outcome of the assumed underlying probability distribution.

An alternative could be to increase the size of TI and hence create additional possibilities for matching events in the TI. However, finding/generating a suitable TI is already the biggest challenge and strength of MPS simulation. The larger TI should still convey the same geology as before but with increased variability, which is not trivial.

We hope this sufficiently answers your question. We will try to rewrite the section to emphasize what exactly constitutes a simulation artifact.

RC2: “Why do the realisations deviate from the TI? “

Following from the above we hope it is clear that realization will always deviate from the TI. It should not be the same. The only place we might expect to have a huge overlap between the TI and the realizations is the area from which the TI is derived. Since the TIs are also in the simulation domain the correspondence between the two might be something to include in the revised manuscript.

The TI represent an outcome of the probability distribution we wish to sample from. The goal is to simulate new realizations that has the same multipoint statistics, but not the actual structures themselves.

RC2: “The non-stationarity of the TI is mentioned but I don’t understand what this means.”

The MPS simulation algorithm is expecting the same spatial variation in the whole training image. A training image that is stationary provides exactly that. For instance, postglacial sediments are only found at the top of TIs in the current study. When the algorithm searches for matching events containing postglacial sediment, matches can then only be found in some specific location. To be more technical, for a process to be stationary, all its statistical properties must be independent of spatial location. This is clearly not the case for a TI built on geology and redox for that matter. Both are extremely non-stationary by nature. Different processes shape the subsurface and it is not providing the same statistical properties at all locations. The issues of non-stationarity in MPS are discussed in detail in Mirowski et al. (2009). Another point is that issues with non-stationarity can be remedied with large amounts of conditional data (see e.g., Barford et al. (2018) or Vilhelmsen et al. (2019)).

Should we perhaps elaborate this within the manuscript? We would argue that for most (geo)statisticians the term is well known. So, this will mostly be of value for people unaware of what exactly non-stationarity is. Another problem is the general length of the manuscript as we try to combine the work of several disciplines (geochemistry, geology, geophysics, geostatistics) we have chosen some areas to focus on while other are left for the reader to delve into.

RC2: "It is suggested that artifacts could potentially be removed through better parametrization, but why would that be, and if so, shouldn't you have attempted to do some parameter 'tuning' as part of this work? "

From our answers above we hope to lift the lid on why parameterization of MPS simulation algorithms is not straightforward. Parameterizing the algorithm depends on 1) the conditional data events available in the TI (its size, variability and stationarity), 2) computational demands and 3) ultimately if the realizations satisfy the variability that is expected within the training image. We focused more on later part from a qualitative perspective but can also include some quantitative measures also. By going too much into detail with parameter optimization we are afraid to divert the attention away from the core message of the paper.

RC2: "I understand that the artifacts are basically being averaged out over multiple realisations, and I think if the main aim was to produce best estimate and associated uncertainty (entropy) of the geology and redox (Figure 11), then the occurrence of artifacts would be less of an issue. However, if the aim is also to provide realisations as input for transport and fate modelling of nitrate, then I would think the artifacts could become much more of an issue, especially as flow and solute transport will depend non-linearly on those realisations. It is argued that for hydrological modelling at catchment scale, the geological artifacts will have limited effect, which may be true, but I'm less convinced the same is the case for nitrate transport, especially given the redox artifacts."

You are completely right here. This will remain an assumption on our part. We do not know to which extent these artifacts affect subsequent hydrological models. The logical next step and what we are currently working on is to explore how these MPS models of the subsurface architecture affect hydrological models. If these redox artifacts are significant, it is possible and trivial within the current workflow to e.g., enforce that below a certain depth only reduced redox conditions would occur.

RC2: “2. The joint simulation requires a bivariate training image (TI) for geology and redox to be developed. I understand how the geological TIs were developed, but I find it less clear how the redox TIs were produced, who produced them and how the bivariate/joint nature of the TIs are specified. I think this could be better explained.”

In the current study, the geological training images were developed primarily by a geologist and the redox training images by a geochemist. We agree that the description of the work carried out in constructing the redox training image is weakly documented. We will try to describe the process and choices made in more detail in the revised manuscript.

RC2: “3. For the case study, two independent bivariate TIs are developed, one representing the Quaternary sequence and one representing the buried valley. It is assumed that the delineation of these geological elements is known in the domain (i.e. no uncertainty as to whether a voxel is Quaternary or buried valley). But what is this delineation based on and with what certainty can this be done?”

The delineation is based on geological interpretation. At the ground surface this interpretation is primarily guided by topographic information combined with the surface geology maps. At depth borehole information and geophysical data (tTEM, SkyTEM etc.) provides spatial information about the boundaries between the geological elements. Knowing the geological processes and the depositional setting from neighboring areas aids this delineation as well. You raise an interesting question regarding the lack of uncertainty for this boundary. We have discussed this internally within the author group. Clearly there is some uncertainty attributed to the location of these boundaries.

The main question is how one can quantify this uncertainty. Also, one must find a way of incorporating these uncertainties in the simulation results. Finally, the effect on the realizations of having such an uncertain boundary must be assessed in comparison to a static boundary. To answer these questions in depth is beyond the scope of the current study. One idea that we would like to follow is to attribute the interpreted boundaries with a quantitative uncertainty based on the interpreter's qualitative uncertainty. By doing so we could simulate several boundary configurations prior to modeling. A set of simulation grids could then be produced that for which we generate one realization. The resulting set of realizations would then satisfy the independence between the geological elements and have a quantitative representation of the uncertainty of this boundary. Alternatively, there is also the possibility to, in direct sampling, simulate with an auxiliary probability grid covering the simulation grid telling which TI to use depending on spatial location. However, this would break the independence between the geological elements as conditional voxels from the buried valley would be included in conditional events for the Quaternary sequence.

RC2: "4. I can't really work out what the influence and significance of the TIs and the conditioning data are for the results. I think it would be relevant to include a discussion on the value of the information used. Given the large amount of conditioning data, does the TI become less important? Would the results be significantly different if you just used the same TI for both the geological elements? What is the effect of the soft data on the result? It would be interesting to see what the results look like if you excluded these. Except for the surface geology, the soft data looks quite uninformative."

Good point. It not straightforward to assess the value of different types of information. Also, because MPS tends to underestimate the importance of soft data compared to hard data. Clearly when looking at the entropy of the final models compared with the soft data, the TI provides a lot of information to the system. We discussed to include prior realizations (no conditioning data) to show the value of adding information to the system. Maybe the TI provides too much information in the current setup. We

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will include a section discussing the value of information for the simulations. It is an important topic.

RC2: “5. It is not clear to me exactly how topography is used to inform soil moisture when deriving soft data for redox conditions. L365 just states how slope/topography affect moisture in general (it sounds like a TOPMODEL type of approach?). I think further explanation is required here. “

The slope is used as a surrogate for moisture. Not to inform soil moisture content. At the Quaternary sequence, we have wells that can assist in translating the surface geology map into probabilities for redox conditions. This is done simply by counting the occurrences of different redox conditions associated with the surface geology conditions. There are too few redox wells available in the buried valley to perform a similar translation. One solution would be to use the probabilities derived for the Quaternary sequence directly in the buried valley. However, we know that topography is coupled to soil moisture content. Since the slope of the buried valley is much flatter, we assume that soil moisture is different in this element and hence scale the probabilities obtained in the Quaternary sequence such that the buried valley has a lower probability of oxic conditions at the surface. This is our justification for changing the probabilities between the two elements.

RC2: “6. Figures: The 3D figures look impressive, but there is a lot of them, and I think they are quite complex, and the colour choices make them not so easy to ‘read’ (especially the small ones). I wonder if some of the figures would perhaps be more illustrative in 2D rather than 3D. I don’t think Fig 5 works very well as a 3D figure, and in Fig. 6 it is difficult to see that tTEM actually only covers part of the simulation grid. In Figure 1a it took me a while before I realised that the blue, black and red lines where actually the TEM and ERT data points. In Figure 7 the colours are difficult to distinguish in the histograms and it looks like there is a shade of blue in Fig 7a that is not in the legend.”

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The other reviewer also had some remarks to the colormap. We intend to change the colormap to have more distinctive colors. We understand your point regarding figure 5. Conversely, we argue that for consistency between the figures it is better to keep figure 5 as an oblique 3D figure. In order to help better show the extent of the simulation grid, we intend to add an opaque version of the simulation grid to figure 6 similar to what is done in figure 5. The problems of figure 7 should be solved when another colormap is chosen. The apparent different shade of blue is probably due to transparency in the histogram. The colors should be identical. In figure 1a we intend to change the legend to better describe the geophysical data.

RC2: "7. Overall, I think the paper is well-written, but there are places where I find the presentation of the material unclear and confusing and where more explanation would be helpful (particularly section 6 and 7). I appreciate that this is not helped by the fact that I'm not so familiar with the MPS method."

Thank you very much. We will go through section 6 and 7 and try to rewrite them. As many readers of HESS would probably be unfamiliar with MPS we will try to elaborate on some of the concepts that might be confusing from an outsider.

Summary of intended changes for new manuscript version based on the above major comments:

- Calculate correspondence between TI and realizations in places where the TI corresponds is situated within the training images - Maybe introduce quantitative measures for realization performance if it does not divert the core message of the paper. - Better description of the process behind both geology and redox TI construction. Focusing on the specific choices during the process. - Include a section on the value of different types of information for the geostatistical simulations - Change colormap for geological realizations. - Revisit section 6 and 7 and rewrite passages that might requires too much background knowledge on MPS.

We intend not to elaborate on the minor comments in the discussion phase but will take these into account in the revised version of the manuscript.

On behalf of myself and the co-authors

Rasmus Bødker Madsen

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