3D Multiple-point Statistics Simulations of the Roussillon Continental Pliocene Aquifer using DeeSse (Valentin Dall'alba et al)

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Anonymous Referee #1 (24 May 2020) :

General comments :	**Responses :**
This manuscript provides an improvement of the MPS implementation through the direct sampling algorithm, in order to design a method for the reconstruction of aquifer heterogeneity at scale lengths of tens of kilometers.	More precisely, the aim of the paper is to present a workflow allowing to apply the direct sampling technique to simulate aquifer heterogeneity at the regional scale. We do not improve the actual implementation of the MPS kernel. We employ the direct sampling MPS kernel into a global workflow.
Overall, the work is interesting and deserves publication. The paper is generally well organized and written, but it can be improved following the suggestions given in the specific comments # 1 and 6. Some other weak scientific flaws can be fixed with a moderate to major revision.	We are thankful to the reviewer for his/her overall evaluation and detailed editing of the paper. This is helping to improve the manuscript and clarify some aspects. Below we discuss more precisely the different issues raised by the reviewer and how we plan to adjust the paper in consequence.
Specific comments :	**Responses :**
1. The abstract is a long summary of the work, but it does not give a precise and clear image of the innovative content of the work. I think that it should be shortened and focused in a more appropriate way. [...]	We agree that the abstract was long and maybe not sufficiently focused on the core of the paper. We propose a revised version that has been shortened. We tried to better highlight the novel aspects of the methodology. The proposed new abstract is the following : "This study introduces a novel workflow to model the heterogeneity of complex aquifers using the multiple-point statistics algorithm DeeSse. We illustrate the approach by modeling the Continental Pliocene layer of the Roussillon's aquifer in the region of Perpignan (southern France). When few direct observations are available, statistical inference from field data is difficult if not impossible, and

	traditional geostatistical approaches cannot be applied directly. On the opposite, multiple-point statistics simulations can rely on a conceptual geological model provided using a training image. But since the spatial arrangement of geological structures is often non-stationary and complex there is a need for methods allowing to describe and account for the non-stationarity in a simple but efficient manner. The main aim of this paper is therefore to propose a workflow for these situations. The workflow is based on the direct sampling algorithm DeeSse. The conceptual model is provided by the geologist as a two-dimensional non-stationary training image (TI) in map view displaying the possible organization of the geological structures and their spatial evolution. To control the non-stationarity, a 3D trend map is obtained by solving numerically the diffusivity equation as a proxy to describe the spatial evolution of the sedimentary patterns, from the source of the sediments to the outlet of the system. A 3D continuous rotation map is estimated from inferred paleo-orientations of the fluvial system. Both trend and orientation maps are derived from geological insights gathered from outcrops and general knowledge of processes occurring in these types of sedimentary environments. Finally, the 3D model is obtained by stacking 2D simulations following the paleo-topography of the aquifer. The vertical facies transition between successive 2D simulations is controlled partly by the borehole data used for conditioning. But we also account for vertical probability of transitions derived from the borehole observations by simulating a set of conditional data points from one layer to the next. This process allows us to bypass the creation of a 3D training image which may be cumbersome in some situations while honoring the observed vertical continuity.”

[...] Moreover, a similar comment applies to the introduction, which describes general properties of MPS, but does not properly introduce the specific methodological question which is faced with this work. The description given at lines 70 to 75 is not very exciting and informative. In my opinion, most of the material in section “3.1 Overview” should be anticipated in the introduction, in order to give a better presentation of the innovative character of this work at the very beginning of the paper.	Similar to the abstract, we propose to reconsider the text as suggested by the reviewer to provide a clearer outline of the approach in the introduction. We will try to emphasize more clearly the novel aspects of the approach. As suggested by the reviewer we also proposed to add some more information about the motivation of the approach and an overview of the workflow in the introduction. The revised text will be placed after the presentation of the MPS methods and will be the following: “The choice of a simulation technique to model an aquifer at a regional scale depends from different factors. One important aspect is the amount of data available. When the amount of data is large, it is possible to infer rather accurately the statistics describing the spatial variability from the data. Probability distributions about the different rock types, variograms, and spatial trends can be directly estimated and used in the simulation process. This situation often occurs in the mining industry for example where very large number of drill holes are made during the exploitation of an ore deposit. The situation is very different in other situations, such as the Roussillon plain, where only a few boreholes are available for a large study area. It becomes then difficult if not impossible to estimate accurately those statistical parameters from the data set. One has then to rely more heavily on indirect data, geological concepts, and analogy with other sites. In these situations, one could borrow statistical distributions, variograms and orders of magnitude of correlations lengths from data bases of similar environments such as those developed by \citet{colombera2012database}. The issue with that approach is that the simulations may be constrained only by a few data points and therefore the final variability among the simulations will be excessively large and the geological features will not be properly represented because the field data will not compensate the lack of geological concept in a variogram based geostatistical approach. An object based method would better respect the geological knowledge because the user will have to explicitly define the shape of the

objects, and this approach could be an interesting solution for these situations with an important data gap. But here, we rather consider the use of MPS. As for the object based approach, it allows integrating directly geological knowledge in the stochastic simulation process.

Another very important aspect to take into account at the regional scale are the statistical non-stationarities resulting from geological processes such as the location of the sources of the sediments, their transport, deposition, and so on. The application of MPS to a real case requires therefore more than just an efficient MPS code and a good training image. It requires also to develop a methodology and a workflow to account for all those aspects.

The aim of this paper is therefore to introduce such a global workflow allowing to incorporate most of the available geological knowledge into a plausible heterogeneity model and to illustrate the method on the Roussillon plain. The workflow is generic and can be applied to any other case where the available data are scarce compared to the geological knowledge. The workflow includes a series of steps that are described in detail in the paper. Based on the borehole and geological knowledge of the site, a plan view non-stationary training image displaying the main sedimentological features is designed. In this paper, we limit ourselves to the construction of a 2D training image since there are many situations in which the cross sectional view at the scale of the aquifer is much less well known than the expected spatial organization of the sedimentary layers on a 2D horizontal plane. The vertical transitions are controlled using probability of transitions derived from the boreholes. To control the lateral transitions and non stationarity, 3D auxiliary maps representing a proxy of the evolution of the system from the source of the sediment to the output are modeled by solving a diffusivity equation. The boundary conditions imposed to the diffusivity equation allow to account for the paleo-input zones and the lateral geometry of the aquifer. In addition, the proposed workflow accounts for the paleo orientations of the sedimentary system

	and its related uncertainty as inferred from field observations. The paper shows that such an approach can be efficient to simulate realistic alluvial systems matching the conceptual knowledge of the system.”
2. For a long part of the manuscript, it was not clear to me whether the TIs were horizontal maps or vertical cross-sections.	The paper already indicates, for example in lines 168-169, that the training image represents the expected pattern in a layer of the same age of deposition. We thought that this was clear enough. But to make the point clearer, we plan to provide the information earlier in the abstract and in the text to ensure that this is clear from the beginning. We plan to correct the legend of figure 2 to clarify the TI orientation : “**Horizontal TIs** associated with their corresponding 2D MPS simulations.” And modify lines 166-167 to clarify the fact that the TI is a horizontal representation of the system : “The TI used for the Continental Pliocene layer is a 2D non-stationary **conceptual plan view of an alluvial system** composed of 6 sedimentary facies.”
Moreover, the way in which 2D horizontal maps are used along the vertical direction should be better analysed. For instance, it would be useful to draw some vertical cross-sections in order to show the effects of the two simulation sets (with and without vertical sampling).	We agree with the reviewer and propose to introduce a new figure representing cross-sections of simulations with and without the sampling approach in order to effectively visualize its effect. This new figure 11 is presented at the end of this document. We also add a small description in section 4.4 : “The impact of the sampling approach can also be easily observed when studying vertical cross-sections along the x and y axis in the transformed grid space (Fig. 11). In Fig. 11a the channels created by the stacking of the braided/meandering facies are vertically disconnected from each other. The impact of the sampling approach that leads to the creation of vertically connected objects can be observed in Fig. 11b. By opposition to the simulation that is not using the sampling strategy, it is now possible to observe "channels like"

	cross-sections in the simulation output.”
In fact the analysis shown in figure 10 is not clear enough.	We propose to add some information on the dissimilarity index beginning at line 373 : “To quantify the impact of the vertical sampling strategy, following previous authors, we compared the distributions of the vertical runs (Mood, 1940, Boisvert et al 2007). To compute this indicator, the 3D grid is decomposed as a set of vertical columns of voxels. A vertical run is then defined as the length of a succession of the same facies values preceded and succeeded by a different facies. By computing the run length on all the columns for a given facies, one can compute the empirical distribution of runs for this facies. The same operation is conducted for all the facies. In addition, these empirical distributions are also computed on the borehole data. We then compute dissimilarity indices between the simulated and observed distributions for all the facies using a normalized euclidean distance. The closest to zero the dissimilarity value is, the more identical the distributions are and reciprocally (Fig. 10b). The alluvial fan facies is here not represented, because it is under-represented in the hard data set and a reference distribution cannot be inferred from it.”
3. Section “3.2 Hard data set” could be improved. (a) There is some confusion between electrofacies and sedimentary facies.	We understand the confusion between the two terms. We propose to modify the paper in order to use only the term **sedimentary facies**, which is more appropriate.
(b) And what about hydrofacies, which are ultimately the most important for hydraulic conductivity?	The reviewer raises an interesting remark. The main answer to this question is that two sedimentological units may have similar hydraulic conductivities but very different geometrical shapes. If we associate them to the same hydrofacies during the geostatistical simulation procedure, experience shows that the geometrical shapes of the two sedimentological units gets mixed and looses consistency. This is why, it is often better to model first the sedimentological units and then fill them with hydraulic properties.

	In addition, this process allows to account better for the hard data descriptions and the indirect geological knowledge and sedimental history of the area.
(c) What about lithological logs? Usually they are available if a borehole is drilled for geophysical logs.	The lithological logs are indeed available and used for the sedimentary facies description. We proposed to clarify this point in section 3.2 : "Hard data correspond to field observations assigned to cell values in the simulation grid. The hard conditioning data set of the Pliocene model is composed of 52 well logs (**lithological**, gamma-ray, and resistivity logs)... By studying the evolution of these response curves coupling with the study of the associated **lithological log**, the sedimentary facies…".
(d) Details about the data set, e.g., position and borehole depth, are missing.	The position of the boreholes was indeed missing. This has been corrected and included in figure 1. We also propose to add some information in the text regarding the borehole data, section 3.2 : "The boreholes are not homogeneously distributed on the plain but are mainly located along the Têt river and in the central zone of the Roussillon's plain (Fig. 1). Their depth range from 20 to 150 m and they are on average 77 m deep."
4. Section "3.3 Training images" is not very convincing. It shows that different TIs give different results and some of these are not appropriate with the geological structure of the study area. This is well known and was clearly proved by some of the authors in previous papers. It is well known that the TI should mimic the structures which are expected in the study area and this should be known a priori from geological studies.	The reviewer is correct in stating that the comparison of several TIs is not novel and should be a rather standard step in any MPS simulation study. We do not claim that this is new. But we think that it is important to discuss that aspect in the framework of non stationary TI and simulations. The simulated patterns are often difficult to predict from the TI alone. Previous publications show that complex simulations can be obtained with very simple training images if proper parametrizations and trends are provided. The simulations will be very different from the TI and therefore the selection of the TI requires some trial and error

	testing. Therefore, we would like to keep that part which is important for the whole procedure in our opinion. This is a step in which several conceptual models can be tested. A point also mentioned by the reviewer and we agree with him on that. Testing various TI is a step of the workflow. We think that at least to illustrate these ideas, this part of the paper can be useful for some readers and should be kept.
Moreover, further details should be given for figure 2a, which shows a strange sedimentary structure (see specific comment# 14).	As presented in the last comment, all of the three TIs described an alluvial system represented with the same main spatial pattern evolution. The different shapes express within a facies through the three TIs are proposed in order to test and represent at different scales different sedimentological hypotheses (eg: whether the braided river deposit cut or not the alluvial fan facies). The facies name must not be taken in a narrow sense as they represent more a location of the depositional environment within the whole alluvial system than a facies description.
I am afraid that the term “braided river facies” is probably used in a non rigorous way. In fact, figure 2b shows the typical structure of a “braided river”, with a great number of intersecting channels.	We disagree with the reviewer but we did not explain clearly enough the reasoning behind this figure. The text will be corrected to better explain the argument. As explained in the previous answer, it is important to consider different pattern configurations in different training images and check how this will be transferred to the regional simulations when combined with non stationarity parameters and trends. This idea led to the creation of three TIs and three different representations of the braided river facies. In the first TI, the braided river facies represents the entire braided channel belt without describing its internal heterogeneity. In the second and third TI, some internal heterogeneity is included in the concept. The reason why the entire braided river channel belt can be considered as one single channel is

	that it happens that there is little potential to preserve low permeability sediments in the braided river channel belt. There is internal heterogeneity in the braided system for sure at a meter scale. But at the reservoir scale, one may consider that the important contrast is the one between the braided river belt and the floodplain. Therefore, it could be reasonable to model the system in that manner.
In other words, areas characterised by meandering rivers show a very strong heterogeneity at relatively fine-scale. This is not properly represented by the TIs.	The same explanation stands for the meandering river, where we decided after detailed discussions with the geologists to represent the meandering river belt and not each individual meanders. This approach is explained by figure 2 e) and is described in detail in the PhD thesis of *Issautier, Benoît. (2011). Impact des hétérogénéités sédimentaires sur le stockage géologique du CO2. University of Aix-Marseille, France : https://www.theses.fr/2011AIX10136*
5. Figure 8 shows that high probability for “floodplain” facies determines approximately linear structures. It seems that these structures separate the similar geometrical features observed for “braided river” and “meandering river” facies. Is this right? This seems to be implicitly stated also in the text.	The geological concept and training images imply indeed an alternation of channels (either meandering or braided) and flood plain. When a hard data indicates the presence of one of the facies, it will impose a high probability of occurrence for this facies at the hard data location, but also upstream and downstream since the channel belts have this rather linear structure. The shape will not be exactly linear because a tolerance is used for the rotation of the channel belts in the plain and the distance between the channels is not constant in the training image. Once a facies is placed, the geological consistency implies that at some lateral distance the other facies (flood plain or channel belt) will have to be present. Therefore, the general pattern identified by the reviewer is correct but the situation is slightly more complex than simple linear trends. We propose to update the text to make the point as clear as possible in the paper.
In individual simulations, “floodplain” facies should be more widely distributed, shouldn’t it? Why these maps show a different structure? Is this due to the constraint given by the elongated	In the individual simulations (for example Fig 7), the flood plain is rather widely distributed. The spacing observed between the river belt in the simulation output (figure 7) corresponds to

features for highest probability of “river” facies?	the indications provided by the geologists on the site. In addition, the overall proportion of flood plain is clearly larger than the channels on every single realization. This is visible in figure 7. In the ensemble of simulations and on the probability maps (figure 8) the flood plain facies has the highest probability of occurrence as compared to the other facies. Therefore, we do not think that the flood plain facies should be more widely distributed.
6. The orientation is missing in all the figures and the scale length is missing in almost all the figures.	Yes we agree. The figures will be modified in order to add scale length and orientation.
Technical comments :	**Responses :**
1. Line 28. The acronym “PC” is used for the Continental Pliocene aquifer. Moreover, in a couple of sentences, I was confused and I read PC as “personal computer”. I understand that “PC” is probably the correct acronym based on initials of French words, but I think that “CP” would be more appropriate as an acronym for the English name.	We understand the possible confusion for the reader, however, this acronym is used by all of the persons that are working in the area. We prefer to keep it for consistency. But we will replace the acronym as much as possible in the revised version of the paper and propose to use the term “Pliocene” when referring to the “Continental Pliocene layer”. We will introduce the terminology at the end of the Geology subsection 2.1 : “In the following, and because we do not consider the deeper Marine Pliocene formations in this paper, we refer to the Continental Pliocene layer and aquifer (usually denoted PC in the area) as Pliocene.”
2. Line 40. Correct “1974)”.	Agree. We will correct this point.
3. Line 58. Correct “Hu, 2008)”.	Agree. We will correct this point.
4. Line 68. Substitute “,” with “.”.	Agree. We will correct this point.
5. Lines 95 to 97. I recommend the authors to carefully follow the international recommendations on the use of SI units and style conventions, in particular the guideline # 12 at the following URL: https://physics.nist.gov/cuu/Units/checklist.htm.	Agree. We will correct this point.

This applies also to other parts of the manuscript.	
6. Lines 95, 97, 110. Substitute “extend” with “extent” or “extension”.	Agree. We will correct this point.
7. Lines 99, 199, 213, 215, 217, 223-225, 286, 344, 345, 361, 362, 404, 419. I think the use of “meander” as adjective is not correct. I suggest to substitute “meander river” with “meandering river”.	Agree. We will correct this point.
8. Line 104. Substitute “plain itself” with “floodplain”.	Agree. We will correct this point.
9. Line 112. Substitute “in” with “at” before “some locations”. Rephrase “up to 8m higher on average”.	We propose to change the sentence to : “In the 1960s, the piezometric level was on average 8 m higher as compared to the 2012 data and even artesian at some locations.”
10. Line 117. Substitute “of” with “by”.	Agree. We will correct this point.
11. Line 166. It is not clear if the TI is a map in the horizontal plane or a vertical cross-section.	We change it to : “The TI used for the Pliocene is a 2D non-stationary conceptual plan view of an alluvial system composed of 6 sedimentary facies.”
12. Line 171. Which is the direction of the x coordinate axis?	The TI is not spatially oriented, however, the x-direction can be assimilated to the east-west direction on the grid.
13. Lines 196-197. Clarify the expression “By studying the evolution of these response curves”.	We propose to reformulate the expression as follow : “By analyzing the gamma-ray and resistivity responses at a certain depth coupling with their vertical evolution, it is possible to identify and assigned a sedimentary facies to a certain depth range.”
14. Line 212. The expression “an analogue river system from northern Italy” does not provide a	We agree with the reviewer that the expression “an analogue river system” can be misleading and lack precision. We used satellite images of

useful information. Which river? Which kind of geological setting? Moreover, from figure 2a, the braided river facies cover an extended area and does not properly represent the internal heterogeneity of a braided river system.	the Tagliamento river, which is located in Northern Italy near the town of Udine and close to the Slovenia border to create the first TI. We propose to change the description line 212 in the new version of the article : "The first TI (Fig. 2a) is created based on visual interpretation of satellite images of the Tagliamento river, which is located in Northern Italy near the town of Udine and close to the Slovenia border. The entire channel belt is considered as the deposition zone. Moreover, this TI neither represents the small scale internal structures of the river deposits nor the levee structures." As for the comment on the "braided river facies", this point is already answered above within the specific comment 4.
15. Line 216. Substitute "meander objects" with "meanders".	Agree. We will correct this point.
16. Lines 285-286. Why "the best way to control the vertical continuity was to sample only from three facies"? Can you comment on this and explain this result?	Since the "floodplain facies" is the most frequent, sampling the facies at random location leads to an over-representation of the flood plain and tends to bias the MPS simulations. After some tests, it appeared that the easiest way to control the connectivity of the objects of interest was to sample only those facies (alluvial fan, braided and meandering river). We also decided to not sample the levee and crevasse splay facies in order to avoid constraining the whole structure of the fluvial objects too heavily. We propose to add these explanations in the revised version of the manuscript.
17. Line 319. Substitute "doesn't" with "does not".	Agree. We will correct this point.
18. Line 340. Substitute "are" with "is".	Agree. We will correct this point.
19. Line 385. Add "a" before "complex".	Agree, we change the end of the sentence to the plural form : "...for the simulation of complex heterogeneous

	aquifers.”
20. Lines 401 to 403. This remark is not so evident from the analysis of the results.	We proposed to clarify the explanations of figure 10 in section 4.4 and cite this figure in lines 401-403. Moreover, a new figure presenting cross-sections through the simulation with and without the sampling approach will be introduced in the revised version of the paper. The figure will clarify the effect of the sampling approach on the vertical connectivity of the river beds.
21. Line 495. Erase “Tectonophysics”.	Agree. We will correct this point.
22. Figure 3. Substitute “c)” with “b)”.	Agree. We will correct this point.

New figure 11 :