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Discussions

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Interactive comment on "A new multi-variable benchmark for Last Glacial Maximum climate simulations" *by* Sean F. Cleator et al.

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We thank Michel for his comments on the paper and are glad to have the chance to respond to them.

Mathematical details of the technique applied in this study are available in Cleator et al., 2019a. This is an arXiv preprint. It is not clear whether the latter is intended for a peer-reviewed journal or whether it was part of a thesis examination.

Response: This article is currently in review with the Journal of Advances in Modeling Earth Systems. As a result of the review process, it was pointed out that the Gaussian correlation function we used did not yield a full rank matrix; we have therefore moved to using a modified Bessel function that closely matches the behaviour of the

original Gaussian function and yields a correlation matrix that is full rank and positive. We have checked that this change does not make a substantial difference to the global reconstructions presented here (although it changes some numbers slightly, and we have amended the text to reflect this) and does not change the conclusions of our paper. The revised method paper is available from arXiv (arXiv:1902.04973v2, https://arxiv.org/abs/1902.04973v2) and we hope will soon be available in JAMES. We have updated the figures and the text here to reflect the use of the revised function.

There are a number of points in this approach which deserve discussion. For this reason it would have been better to see these method details in the Climate of the Past paper, so that the paper, the review, and possible responses constitute a self-contained contribution.

Response: We wanted to focus the discussion here on the results (i.e. the reconstructions of LGM climate) rather on the mathematical details of the method. These details should shortly be available in JAMES and are given in the pre-print article. However, we agree that it would be worth expanding the section on the application of the data assimilation method and the choice of length scales (section 2.4) to provide more details. We propose to modify this section as follows:

Variational data assimilation techniques provide a way of combining observations and model outputs to produce climate reconstructions that are not exclusively constrained to one source of information or the other (Nichols, 2010). We use the 3D-variational method, described in Cleator et al. (2019a) to find the maximum a posteriori estimate (or analytical reconstruction) of the palaeoclimate given the site-based reconstructions and the model-based prior. The method constructs a cost function, which describes how well a particular climate matches both the site-based reconstructions and the prior, by assuming the reconstructions and prior have a Gaussian distribution. To avoid sharp changes in time and/or space in the analytical reconstructions, the method assumes that the prior temporal and spatial error correlations are derived from a modified Bessel function, in order to create a climate anomaly field that is smooth both from month to

month and from grid cell to grid cell. The degree of correlation is controlled through two length scales: a spatial length scale that determines how correlated the error in the prior is between different geographical areas, and a temporal length scale that determines how correlated it is through the seasonal cycle. The site-based reconstructions are assumed to have negligible correlations at these space and time scales. The maximum a posteriori estimate is found by using the limited memory Broyden-Fletcher-Goldfarb-Shanno method (Liu and Nocedal 1989) to determine the climate that minimises the cost function. A first order estimate of the analysis error covariance is also computed. An observation operator based on calculations of the direct impact of [CO2] on water-use efficiency (section 2.3) is used in making the analytical reconstructions. The prior is constructed as the average of eight LGM climate simulations (section 2.2). We use an ensemble of different model responses to the same forcing to provide a series of physically consistent possible states, which can be viewed as perturbed responses and provide the variance around the climatology provided by the ensemble average. The prior error correlations are based on a temporal length scale (L_t) of 1 month and a spatial length scale (L_s) of 400km. Cleator et al., (2019a) have shown that a temporal length scale of 1 month provides an adequately smooth solution for the seasonal cycle, both using single sites and over multiple grid cells, as shown by the sensitivity of the resolution matrix (Menke, 2012; Delahaies et al., 2017) to changes in the temporal length scale. Consideration of the spatial spread of variance in the analytical reconstruction shows that a spatial length scale of 400km also provides a reasonable reflection of the large-scale coherence of regional climate change.

Additional references: Liu, D. C., & Nocedal, J. (1989). On the limited memory BFGS method for large scale optimization. Mathematical Programming, 45 (1), 503–528. doi: 10.1007/BF01589116 Delahaies, S., Roulstone, I., & Nichols, N. (2017). Constraining DALECv2 using multiple data streams and ecological constraints: analysis and application. Geoscientific Model Development (Online), 10 (7). doi: 10.5194/gmd-10-2635-2017 Menke, W. (2012). Geophysical data analysis: Discrete inverse theory (Matlab 3rd ed.). Cambridge, Massachusetts: Academic Press.

Unlike what (roughly) obtains when using time series of a numerical weather prediction system, there is a priori no guarantee that the covariance matrix of a multi-model ensemble produces modes which satisfy "physical consistency". Why would we expect that the inter-model differences provide knowledge about how different variables should co-vary?

Response: Our argument here is that the average response of all the models gives a measure of climatology. Numerical weather prediction uses ensembles of perturbed responses to provide a series of physically-consistent possible states, although there are examples of using multiple models to form an ensemble (see e.g. Johnson and Swinbank, 2009 - https://rmets.onlinelibrary.wiley.com/doi/pdf/10.1002/qj.383). Here we use an ensemble of different model responses to the same forcing, which can be viewed as producing perturbed responses to the general climatology. We have added a sentence in the method text (given above) to make this argument clearer.

In principle, a "prior" encodes what we a priori believe the climate could be. The authors have then chosen to mask regions with little update by observations, and leave visible the grid points where the observations have seriously shifted the prior. This seems at first sight reasonable because the idea is to focus on the pollen reconstructions and not on the PMIP3 output. Yet, at face value, this approach is inconsistent with a Bayesian interpretation. Grid points of strong update are associated, in the Bayesian interpretation, with a very small marginal likelihood (a wrong prior means a wrong model).

Response: We are starting from the assumption that the pollen-based reconstructions are more likely to be correct than the model simulations; but that the model simulations provide us with physically-consistent relationships in space and time (which cannot be obtained from the pollen). This comment is partly due to a misunderstanding about the masking, which is in fact determined by the variance rather than the absolute change. Only areas with an improved variance are shown (i.e. left unmasked). This means that the likelihood that these reconstructions represent the true climate is significantly

improved from the prior. This only happens if the variance in the observations is small and the variance in the prior is big. By using both local and global measures of the variance in the prior, we avoid a situation where the variance in the prior is small but shows a different signal from the pollen-based reconstructions. We will expand the text to make this clearer (lines 277-278) as follows:

The reliability of the analytical reconstructions was assessed by comparing these composite errors with the errors in the prior. We masked out cells where the inclusion of site-based reconstructions does not produce an improvement of > 5% from the prior. Since this assessment is based on a change in the variance, rather than absolute values, this masking removes regions where there are no pollen-based reconstructions or the pollen-based reconstructions have very large uncertainties.

To what extent should we be concerned that the posterior variance remains influenced by the prior variance? Indeed, mathematically, the posterior variance is bounded by the prior variance, which âĂŤ if we admit the models are really off âĂŤ is meaningless.

Response: The posterior variance is influenced (though not bounded or limited by) by the prior variance. However, since areas that have a small change to prior covariance are masked out, only areas with pollen-based reconstructions with low variance are used in the reconstruction. Hence, the prior variance only influences the posterior variance in areas that are well constrained by observations. Furthermore, since the prior variance is based partly on the global variance for each variable, the only way to have a large prior variance affecting the posterior variance is for all models to agree well globally and locally and the observation to have a low variance such that the posterior variance has improved upon the prior variance change by over the 5% cutoff. We agree that the choice of the cutoff is somewhat arbitrary (as we state in the discussion section,(lines 406-412), though guided by examination of the impact of this cutoff on the reconstructions, and that it would be useful to develop an objective way of determining an appropriate limit. We will expand the discussion further, to suggest ways forward here (lines 406-412) as follows:

We have used a <5% reduction in the analytical uncertainty compared to prior uncertainty to identify regions where the incorporation of site-based data has a negligible effect on the prior as a way of masking out regions for which the observations have effectively no impact on the analytical reconstructions. The choice of a 5% cut-off is arbitrary, but little would be gained by imposing a more stringent cut-off at the LGM given that many regions are represented by few observations. A more stringent cut-off could be applied for other time intervals with more data. We avoid the use of a criterion based on the analytical reconstruction showing any improvement on the prior because this could be affected by numerical noise in the computation. Alternative criteria for the choice of cut-off could be based on whether the analytical reconstruction had a reduced uncertainty compared to the pollen-based reconstructions or could be derived by a consideration of the condition number used to select appropriate length scales.

To what extent the prior covariance (link between different variables) may still be trusted at all if the models are so wrong? This remark strengthens the original concern about the physical meaning of the covariance matrix, even when the prior is only mildly updated. What is the advantage of this approach over a mere Gaussian interpolation (flat climate prior), which in this case might turn out to be more reliable and free of the dubious claim of "physical consistency"?

Response: We acknowledge that the climate models may not be correct, for example because the LGM simulations do not include all of the necessary forcings or show weak responses to these forcings. However, analyses of the PMIP simulations indicate that while the models show differences of both magnitude and sign in some regions, the overall LGM to present change is broadly consistent with what we know from observations. It is worth pointing out that many of these regional problems are associated with model dynamics rather than thermodynamics, which suggests that the models can be used to ensure physical consistency between surface variables. We try to overcome the problem of "all models being consistent but wrong" at a regional scale by combining global and local uncertainties to produce the uncertainty on the prior. In revising

the section describing the variational approach (see above), we have tried to make our logic clearer here.

Were the length scales tested by some form of cross-validation (e.g. leave-one-out), or were they merely chosen because they are a priori reasonable?

Response: We did not use cross-validation to evaluate the choice of length scales, but instead we based the choice of length scales on sensitivity experiments (as described in the arXiv pre-print). Effectively we ran a series of tests to see how different choices affect the resolution matrices and the condition number. We selected a spatial length scale that provided a reasonable reflection of the large-scale coherence of regional climate change and also ensured that the covariance matrix was well-conditioned for inversion, and a temporal length scale that limited overlap between successive months. The selected length scales seem reasonable; for example, the spatial scale corresponds to a situation where there is little overlap between data points assuming an average catchment size for the pollen records on which the original reconstructions were based. Similarly, the selected temporal length scale produces plausible-looking seasonal cycles of temperature. We have expanded the text describing the application of the variational method (see above) to clarify how the length scales were chosen based on these sensitivity tests and a post-hoc evaluation of plausibility.

The arXiv paper provides the definition of the moisture index. It should be repeated here (moisture index is currently introduced l. 297 without definition)

Response: We apologise for not defining MI at first use; it is in fact currently defined at line 155. In the present context the reference to MI is inappropriate because the text refers to a generic control by moisture availability rather than a specific index. We also note there was a crucial comma missing in this sentence! We will alter the text here to read: which is generally taken into account by process-based ecosystem models, but not by statistical models, using projected changes in vapour pressure deficit or some measure of plant-available water

C7

The authors should consider providing a link to supporting code. The maps are currently provided as University of Reading dataset (with a doi) but its lifecycle is detached from the present contribution. A dataset consistent with the current Climate of the Past submission, reflecting a possible response to concerns of the reviewers, might best be included as supplementary information. Have we lodged code somewhere?

Response: The data used to generate the maps are lodged at the University of Reading repository, with a DOI. This allows external users to generate their own maps and their own analyses using the reconstructions. A revised version of these data, reflecting minor changes in the data as a consequence of using a Bessel function, has now been lodged at the repository. The two data sets are linked, so that external users are directed to the updated version of the data set. We do not envisage any changes to the data set as a result of review of this CoP submission, but if there are further changes to the data set then the current data set can be updated and again linked. Thus, the data provided in the repository are indeed constantly linked to the lifecycle of the product. The code used to generate the reconstructions has been lodged at Zenodo, and we will provide the DOI for this code in the revised ms. We will add a data availability section to the ms as follows: Data availability: the gridded data for the LGM reconstructions are available from http://dx.doi.org/10.17864/1947.206; the code used to generate these reconstructions is available from (10.5281/zenodo.3445166).

It is important to distinguish the notion of variance from the notion of uncertainty. They are not synonymous. Variance describes the second momentum of a distribution; uncertainty is a reference to an identified lack of knowledge. Only when the distribution is assumed reflects our knowledge of a given quantity is it legitimate to identify both.

Response: We agree that the use of terminology here is inaccurate and we need to be more precise. However, uncertainty is not simply an identified lack of knowledge! It is also used to refer to the limits on the precision of knowledge (as in the case where we talk about the uncertainties attached to a pollen-based climate reconstruction, which are partly a function of our ability to define precise relationships with existing training

data sets). We have corrected the ms throughout to ensure that we use variance and uncertainty appropriately. We have made the following specific changes: l.34 error changed to uncertainty l.134 error changed to uncertainty l.268 error changed to variances l.269 error changes to covariances l.272-278 error changed to variance l.282 error changed to variances l.283 error changed to variances (We have also changed this for Figure 3 in the caption list section) l.147 uncertainty change to variances Figure 2 caption, uncertainty changed to variances Figure 3 caption, uncertainty changed to variances l.406 uncertainty changed to variance

Multi-model ensembles, in general, cannot be said to capture our knowledge of the state of climate at a given time. For this reason, I would argue not to call the PMIP3 covariance a "background uncertainty".

Response: We agree that models are not the only source of information about the state of the climate at a given time, and indeed our approach makes the assumption that the pollen-based reconstructions are more likely to represent the true state of the climate. We agree that the models may be wrong because they do not include all the appropriate forcings, because the response to these forcings is too weak, or because of inappropriate treatment of key feedbacks. We also agree that not all models are equally good (or bad) and that in an ideal world a prior should be reconstructed based only on an ensemble of well-validated models. However, the point of using climate models here is to provide a way of deriving physically consistent relationships between climate variables, given that we do not have reconstructions of all of the seasonal variables everywhere. Furthermore, there are comparatively few LGM simulations available and using a more limited number of "more likely to be correct" simulations to create the prior (and estimate its variance) does not seem to be a good option. In the future, it might be possible to combine PMIP3 and PMIP4 simulations to create a more robust/plausible prior, but this is currently not possible.

The legend of Figure 2 clearly identifies "uncertainties" with "standard deviation of the non-dimensionalised multi-model ensemble" but this seems inadequate to me. Adding

to the confusion, different qualifiers occur throughout the text: "explicit uncertainty" (l. 97), "analytical uncertainty" (l. 406), and, on Figure 3, "grid-based errors in the prior" and "global uncertainty".

Response: We agree that we have not been consistent about the terminology, and particularly the use of terms such as uncertainty, error and variance. We will revise the manuscript so that we are consistent about the terminology, and we will make sure that our use of terms such as explicit uncertainty and analytical uncertainty is clearer for the reader. The changes made are listed in response to the earlier comment about the confusion between uncertainty and variance.

As the uncertainty quantification seems to be a selling point of the present article, the assessment should be more open and transparent about sources of uncertainty, and discuss which of theses sources can be quantified and how. For example, little is said about uncertainties introduced by the CO2 physiological correction. Is it guaranteed to be accurate?

response: There are three basic sources of uncertainty: the pollen-based reconstructions, the construction of the prior, and the uncertainties associated with our implementation of the method. While we have addressed the uncertainties associated with the first two, we agree that the methodological uncertainties were not as well addressed in this paper (although they are discussed in the Prentice et al., 2017 paper from which we derived the CO2 correction approach, and in the arXiv pre-print). The expanded description of the variational method (see above) is now more explicit about potential uncertainties associated e.g. with choice of length scales and cut-offs. For the CO2 correction, we made a series of sensitivity analyses in the Prentice et al. (2017) paper to determine the impact of uncertainties (or errors) in the input parameters. These sensitivity tests showed that the magnitude of the correction was insensitive to the reconstructed temperature, the reconstructed change in temperature relative to the modern reference, or the reconstructed moisture level. The magnitude of the correction is highly sensitive to the level of CO2 specified, but this is well-constrained from the ice-

core records. We will expand the text in the discussion of the CO_2 effect to make this clearer (lines 378-385), as follows:

…. differences in water use efficiency of different PFTs can be almost entirely accounted for by a single equation, as proposed here. Sensitivity analyses show that the numerical value of the corrected moisture variables (MI, MAP) is dependent on the reconstructed values of these variables, but is insensitive to uncertainties in the temperature and moisture inputs (Prentice et al., 2017). The strength of the correction is primarily sensitive to [CO2], but the LGM [CO2] value is well constrained from ice-core records. The response of plants to changes in [CO2] is non-linear (Harrison and Bartlein, 2012), and the effect of the change between recent and pre-industrial or mid-Holocene conditions is less than that between pre-industrial and glacial conditions. Nevertheless, it would be worth taking the [CO2] effect on water-use efficiency into account in making reconstructions of interglacial time periods as well.

The strategy for identifying grid points with little posterior update explained l. 406 is not quite clear. Why not consider a Kullback-Leibler divergence? At the risk of repeating myself, I am concerned about the (meaningless) residual influence of the prior variance and covariance in cases where the prior is effectively discarded by the observations.

Response: As we have explained above in response to the question about masking (and will clarify in the text, lines 277-278), for each variable in each grid cell, we calculate the percentage change of variance between the prior and posterior. We then mask away variables where there is a less than 5% increase in variance. We do not use the Kullback-Leibler divergence approach because this requires the calculation of covariance. However, the two approaches will likely not yield results that are very dissimilar.

This is a minor comment, but the comparison with Goosse et al. 2006 is perhaps slightly misleading. The Goosse et al. purpose was dynamic reconstruction, while the purpose of the present contribution is to provide a diagnostic reconstruction. In

passing, Goosse (2006) did not use a "Kalman particle filter" (whatever it means). Goosse et al. used what they called an "optimal realisation" iteration, which can be interpreted as a highly degenerate form of particle filter. Dubinkina et al. 2011, doi 10.1142/S0218127411030763, adopted a more standard particle filter.

Response: The reference to the Kalman filter is somewhat misleading, although as you point out the approach used by Goosse et al. (2006) can be considered a form of particle filter. Our point here is that filters that select from model output are inherently constrained by the model output, whereas variational approaches can go beyond the values produced by the model. We have changed the wording of the text (line 420-422) to make our main point clearer:

Particle filter approaches (e.g. Goosse et al., 2006; Dubinkina et al., 2011) produce dynamic estimates of palaeoclimate, but particle filters cannot produce estimates of climate outside the realm of the model simulations.

This said, the argument that the variational approach produces maps outside the realm of climate simulations is a double-edged sword. The variational approach assumes Gaussian distributions, and is mathematically equivalent to a Laplace approximation of arbitrary distributions. This is this approximation which allows generating posterior distributions far from the prior. But, in this case, sound Bayesian interpretation should lead us to treat such posterior as utterly suspicious.

Response: It is not clear why a posterior distribution that is far from the model-based prior is utterly suspicious, if being far from the prior reflects the fact that the observational constraints are strong. We are not pretending that there should be equal weight given to the model-based prior and the pollen-based reconstructions, only combining the two and drawing on their individual strengths produces a more reliable estimate of the "true" climate state. Our approach is specifically designed to permit analytical reconstructions that are far from the model-based prior, if this is consistent with the observations and those observations have low variance.

line 384 : It is said that it "would be worth taking [changes in length scales] into account." I would advise either deleting this sentence, or giving more substance to the claim. For example, have you already performed some sensitivity experiments.

Response: The cited text is not talking about changes in length scales, but rather about the necessity to take the CO2 correction into account in making reconstructions of interglacial climates. We have amended this sentence to make this clear, as follows:

Nevertheless, it would be worth taking the [CO2] effect on water-use efficiency into account in making reconstructions of interglacial time periods as well.

Is the very first paragraph really necessary?

Response: Strictly speaking, it should not be necessary, especially for a palaeoclimate audience. However, this does seem to be a point which is largely ignored by many climate modelling centres worldwide, and at least one of the authors (SPH) thinks it bears repeating. We can remove the paragraph if the editor disagrees.

There is room for improving wording accuracy. In what sense is the benchmark "robust" (l. 37) ? l. 97: You write: "explicit uncertainties attached to it". Did you mean "uncertainties explicitly attached" ? Avoid, where possible, the phrase "in terms of" or "means that" (ll. 321 - 326, in particular, need rewording). What is meant by a "statistical reconstruction method" l. 370 (the present exercise is a statistical reconstruction isnt'it ?).

Response: We have been through the manuscript and tightened up the wording. With respect to the specific sentences above, we have made the following changes:

L 37: Thus, the new reconstructions provides a benchmark created using clear and defined mathematical procedures that can be used for evaluation of the PMIP4/CMIP6 entry-card LGM simulations.

L. 97: However, there has so far been no attempt to produce a physically consistent, multi-variable reconstruction which provides the associated uncertainties explicitly.

L 321 et seq.: There are systematic differences, however, between the analytical reconstructions and the pollen-based reconstructions of moisture-related variables (MAP, MI) because the analytical reconstructions take account of the direct influence of [CO2] on plant growth. The physiological impact of [CO2] leads to analytical reconstructions indicating wetter than present conditions in many regions (Figure 5a, Figure 5b), for example in southern Africa where several of the original pollen-based reconstructions show no change in MAP or MI compared to present, but the analytical reconstruction shows wetter conditions than present. In some regions, incorporating the impact of [CO2] reverses the sign of the reconstructed changes. Part of northern Eurasia is reconstructed as being wetter than present, despite pollen-based reconstructions indicating conditions drier than present (both in terms of MAP and MI), as shown by SI Figure SI 3. The relative changes in MAP and MI are similar across all sites (Figure 5c), implying that the analytically reconstructed changes are driven by changes in precipitation rather than temperature.

L 370: Statistical reconstruction methods that use modern relationships between pollen assemblages and climate under modern conditions (i.e. modern analogues, transfer functions, response surfaces: see Bartlein et al., 2011 for discussion) cannot account for such effects.

Figure 5: Shouldn't "pre-industrial reference" be preferred over the vague wording "original" as x-axis label?

Response: We agree that the axis labels on this Figure are not clear. These plots contrast the original pollen-based reconstructions of MI and MAP with analytical reconstructions before (circles) and after (crosses) the CO2 effect is taken into account. We will change the axis labels to read: Pollen-based MI and Pollen-based MAP. We will also expand the caption to make this clearer, as follows:

Figure 5: Impact of CO2 on reconstructions of moisture-related variables. The individual plots show (a) the change in moisture index (MI) and (b) the change in mean

annual precipitation (MAP) compared to the original pollen-based reconstructions for the LGM when the physiological impacts of [CO2] on water-use efficiency are taken into account. The third plot (c) shows the relative difference in MI and MAP as a result of [CO2], shown as the percentage difference between the no-[CO2] and [CO2] calculations.

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