

Collated responses to reviews

Reviewer 1

Comment: clarification of data availability

Response: As the reviewer points out, the pollen-based reconstructions and the climate model simulations underpinning our reconstruction are in the public domain, and the data assimilation methodology is described in detail in another publication. The general approach used for the CO₂ corrections, which the reviewer describes as a significant contribution, was published in Prentice et al. (2017) – although we provide the equations for the implementation of this approach in the current paper in Appendix 1. Therefore, the new results in this paper are indeed the global maps of reconstructed climate variables. These data are archived and will be made publicly available – however, we realise that it may not have been obvious that the citation to Cleator et al. (2019b) represented the reconstruction data set. We have modified the last sentence of the abstract to make it clear that the reconstruction data are available as follows:

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 and are available at DOI:10.17864/1947.229

We have included a Data Availability section in the revised paper:

Data availability. The gridded data for the LGM reconstructions are available from <http://dx.doi.org/10.17864/1947.229>; the code used to generate these reconstructions is available from (10.5281/zenodo.3445166).

Comment: Varying definitions of the LGM

Response: The reviewer indicates that the definition of the LGM used in our paper (21 ± 1 ka) differs from the interval used by Annan and Hargreaves of 21 ± 2 ka, and there is recent work on sea level (Ishiwa et al. 2019) which suggests the ‘real’ LGM was 19.1-19.7 ka, with a plateau prior to this from 20.4-25.9ka. Our choice of this time interval reflects the fact that the LGM is conventionally defined in PMIP at 21 ka and most of the pollen-based reconstructions of this interval included in the Bartlein et al data set are from the 21 ± 1 ka. We are aware that there is still controversy over the timing of the LGM, with both younger and older ages mooted for the actual maximum ice volume/sea-level lowering (see e.g. Peltier and Fairbanks, 2006; Clark et al., 2009; Lambeck et al., 2014). Even the recent work by Ishiwa et al. (2019) points out that the sea level drop after 19.7 ka was only 10m and that there was a long plateau with stable low sea level prior to this and encompassing the 21 ka interval. Since our aim is to produce a data set for benchmarking new PMIP LGM simulations, which will be run with boundary conditions for 21 ka (Kageyama et al., 2017), the exact date of the LGM is therefore not an issue. However, we agree that there is a difference between the true definition of the LGM and the convention used for modelling purposes, and that this is not clear from our introductory text, so we have expanded our definition (line 55 onwards) as follows:

At the Last Glacial Maximum (LGM, conventionally defined for modelling purposes as 21 000 years ago), insolation was quite similar to the present, but global ice volume was at a

maximum, eustatic sea level was close to a minimum, long-lived greenhouse gas concentrations were lower and atmospheric aerosol loadings higher than today, and land surface characteristics (including vegetation distribution) were also substantially different from today.

Comment: Consider how to use new studies published after Bartlein et al.

Response: The reviewer points out that we refer to several new studies since the Bartlein paper on which the analysis is based, and there are more, and that it would be nice to think these could be assimilated into a future dataset to maybe close some of the large ‘no data’ holes in the results. We thoroughly agree that it would be good to plug the gaps, and this will be an effort for the future. The three papers that we cite at lines 361-363 (Flantua et al., 2015; Herbert and Harrison, 2016; Harrison et al., 2016) demonstrate that there are pollen records available that would plug the gaps, but alas do not provide quantitative reconstructions at these sites. The Izumi and Bartlein (2016) paper provides an inversion-based reconstruction for North American – this region is already relatively well covered in the Bartlein et al data set. Similarly Mauri et al. (2015) provide a new gridded reconstruction for Europe – again a region that is well covered in the Bartlein et al data set. However, we are aware of new pollen-based quantitative reconstructions embracing the LGM for individual sites (e.g. in Africa, China, Russia, southern Europe) and compiling these reconstructions would certainly be a worthwhile effort in the future. Our method also lends itself to combining pollen-based reconstructions with other quantitative estimates of terrestrial palaeoclimate, and again this should be something that is done in the future. We have revised the paragraph describing future possibilities to expand the current data set to spell out some of these opportunities more clearly (lines 304-309), as follows:

Some areas are still poorly covered by quantitative pollen-based reconstructions of LGM climate, most notably South America. More pollen-based climate reconstructions would provide one solution to this problem – and there are many pollen records that could be used for this purpose (Flantua et al., 2015; Herbert and Harrison, 2016; Harrison et al., 2016). There are also quantitative reconstructions of climate available from individual sites (e.g. Lebamba et al., 2012; Wang et al., 2014; Loomis et al., 2017; Camuera et al., 2019) that should be incorporated into future data syntheses. It would also be possible to incorporate other sources of quantitative information, such as chironomid-based reconstructions (e.g. Chang et al., 2015) within the variational data assimilation framework.

Additional references

- Camuera, J., Jiménez-Moreno, G., Ramos-Román, M.J., García-Alix, A., Toney, J.L., Anderson, R.S., Jiménez-Espejo, F., Bright, J., Webster, C., Yanes, Y., José S. Carrión, J.S., 2019. Vegetation and climate changes during the last two glacial-interglacial cycles in the western Mediterranean: A new long pollen record from Padul (southern Iberian Peninsula), *Quaternary Science Reviews*, 205, 86-105, <https://doi.org/10.1016/j.quascirev.2018.12.013>.
- Chang, J.C., Shulmeister, J., Woodward, C., Steinberger, L., Tibby, J., Cameron Barr, C., 2015. A chironomid-inferred summer temperature reconstruction from subtropical Australia during the last glacial maximum (LGM) and the last deglaciation, *Quaternary Science Reviews*, 122, 282-292, <https://doi.org/10.1016/j.quascirev.2015.06.006>.

- Lebamba, J., Vincens, A., and Maley, J.: Pollen, vegetation change and climate at Lake Barombi Mbo (Cameroon) during the last ca. 33 000 cal yr BP: a numerical approach, *Clim. Past*, 8, 59-78, <https://doi.org/10.5194/cp-8-59-2012>, 2012.
- Loomis, S. E., Russell, J. M., Verschuren, D., Morrill, C., De Cort, G., Sinninghe Damsté, J. S., ... Kelly, M. A. (2017). The tropical lapse rate steepened during the Last Glacial Maximum. *Science advances*, 3(1), e1600815. doi:10.1126/sciadv.1600815
- Wang, Y., Herzschuh, U., Shumilovskikh, L. S., Mischke, S., Birks, H. J. B., Wischniewski, J., Böhner, J., Schlütz, F., Lehmkuhl, F., Diekmann, B., Wünnemann, B., and Zhang, C.: Quantitative reconstruction of precipitation changes on the NE Tibetan Plateau since the Last Glacial Maximum – extending the concept of pollen source area to pollen-based climate reconstructions from large lakes, *Clim. Past*, 10, 21-39, <https://doi.org/10.5194/cp-10-21-2014>, 2014.

Comment: L59: change to ‘lower, atmospheric aerosol. . .’

Response: We have made this change.

Comment: L321: comma after ‘however’

Response: We have made this change (now line 274).

Response to Review 2

Comment: 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 now accepted for publication in the Journal of Advances in Modeling Earth Systems. As a result of the review process for JAMES, 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 will soon be available in JAMES. We have updated the figures and the text here to reflect the use of the revised function.

Comment: 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 will 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 have modified 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 covariance 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 covariance 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 uncertainty 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 uncertainty 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.

Comment: 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.

Comment: 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 265-271) as follows:

The reliability of the analytical reconstructions was assessed by comparing these composite covariances with the uncertainties 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.

Comment: 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 if we admit the models are really off, 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 have expanded the discussion 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.

Comment: 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 up-dated. 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.

Comment: 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.

Comment: 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: The MI was 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 have altered 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

Comment: 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 have provided the DOI for this code in the revised ms. We have added 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/10.17864/1947.229>; the code used to generate these reconstructions is available from (10.5281/zenodo.3445166).

Comment: 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: 1.34 error changed to uncertainty 1.134 error changed to uncertainty 1.268 error changed to variances 1.269 error changes to covariances 1.272-278 error changed to variance 1.282 error changed to variances 1.283 error changed to variances (We have also changed this for Figure 3 in the caption list section) 1.147 uncertainty change to variances

Figure 2 caption, uncertainty changed to variances Figure 3 caption, uncertainty changed to variances 1.406 uncertainty changed to variance

Comment: 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.

Comment: 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 have not been consistent about the terminology, and particularly the use of terms such as uncertainty, error and variance. We have revised the manuscript so that we are consistent about the terminology, and have clarified what we mean by explicit uncertainty and analytical uncertainty. The changes made are listed in response to the earlier comment about the confusion between uncertainty and variance.

Comment: 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 these 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. We addressed the uncertainties associated with the first two, but 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 have expanded the text in the discussion of the CO₂ 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.

Comment: 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.

Comment. . . 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 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 this 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.

Comment: 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.

Comment: 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.

Comment: 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 is therefore worth repeating.

Comment: 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 isn't 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 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.

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

Response: The axis labels on this Figure are not clear. These plots contrast the original pollen-based reconstructions of MI and MAP with analytical re-constructions before (circles) and after (crosses) the CO₂ effect is taken into account. We have changed the axis labels to read: Pollen-based MI and Pollen-based MAP. We have expanded 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.

Response to review 3

Comment: The paper is quite short and lacks any detailed evaluation of the resultant product. The community's use of this new data product would in my opinion be aided by a more in-depth evaluation of the properties of the reconstruction. It's not clear how important the choices around the assimilation formulation are for the final reconstruction. Specifically the section around lines 268-278 should in my opinion be spelled out and the sensitivity to these choices evaluated.

Response: It is unclear what kind of evaluation of the product the reviewer envisages, given that there is no global ground-truth data set other than the pollen-based reconstructions themselves. We have already pointed out (lines 317-321) that the analytical reconstructions of temperature are close to the Bartlein et al. (2011) data set, both in terms of magnitudes and spatial patterns. The differences between the analytical reconstructions and the Bartlein et al. (2011) reconstructions of moisture variables are a consequence of the fact that statistical techniques based on modern pollen-climate relationships cannot account for CO₂-induced changes in water-use efficiency. In terms of the impact of methodological choices, the major issue here is the choice of length scales. We have made sensitivity analyses to examine the implications of the choice of length scales, and this was discussed in the arXiv preprint. In

expanding the description of the application of variational techniques here (see text in response to Michel Crucifix's review) we have commented further on this.

Comment: The statistical methodology that forms the basis of this study is also not described here but in a arXiv article. I'd like to see more of this brought into the present manuscript to make it self-contained.

Response: This is a point raised by Michel Crucifix in his review. We have now modified the text describing the application of the variational method to include a fuller description of our approach. The full details of the method are now in press in JAMES and we have made the post-review version of this paper available on arXiv.

Comment: Line 127: define MI here.

Response: The reference to MI is inappropriate in the present context 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! In response to Michel Crucifix's review, we have modified this text 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

Comment: Line 209: modelsfor -> models for

Response: We have corrected this.

Comment: Line 252-253: I think it might be appropriate to bring some/all of this methodology into the present text, as discussed above.

Response: We have modified the text here to provide more detail about the method. Please see proposed revised text given in the response to Michel Crucifix's review.

Comment: One question that arises from briefly reading the methodology paper, relates to figure 1 in the arXiv article. Here the assimilation appears not satisfy the pollen-inferred MTCO. Is this because the prior (from the models) is relatively consistent, and so doesn't allow the assimilation to get that cold? Does this happen when applied to the pollen data here?

Response: Figure 1 in the arXiv pre-print does not show a real situation but was designed to illustrate the procedure. In general, the pollen-based reconstructions of MTCO are further away from the model-based prior than summer temperature measures. If the variance in the pollen-based MTCO reconstructions is small, then the analytical reconstructions will be close to the pollen-inferred MTCO. If there is high uncertainty in the pollen-based reconstructions, then the analytical reconstructions are not strongly constrained by these reconstructions and will be further away. This makes intuitive sense because we do not want to rely on pollen-based reconstructions if there is large uncertainty. Thus, it is possible for the assimilation to produce cold results but only if there is tight agreement between the observations about the magnitude of the cooling.

Comment: How do we interpret these choices, given that the climate models themselves could feasibly be systematically biased, e.g. through not including aerosols, or using modern vegetation distributions? How have you addressed the possible systematic bias in the models and hence in your prior?

Response: It is possible that the models show a systematic bias because they do not include all of the appropriate forcings for the LGM climate. We assume that such a systematic bias would primarily influence the magnitude of changes rather than the physical relationship between variables or across space. The presence of a systematic bias is therefore not important because the pollen-based reconstructions effectively correct for any systematic biases in the model-based prior, providing the pollen-based reconstructions have low uncertainty. One of the reasons that we discuss in the paper for adopting a variational technique, rather than some kind of filtering, is that this approach means that the analytical reconstructions can go beyond the range of the simulated climate.

Comment: Line 268-276: This section seems crucial to me, but is not clearly described. Please include the mathematical formulation used and a justification for choices made.

Response: We have expanded the text describing the application of the variational method, including a description of the composite errors. Please see revised text included in the response to Michel Crucifix's review.

Comment Lines 276-278: Do you mean that if the data is too uncertain you mask it based on a 5% criteria? Please could you re-phrase to clarify.

Response: When the change in the variance between the analytical reconstruction and the prior is less than 5%, it does indeed mean that the climate is not well constrained by observations (i.e. that there is high uncertainty in the observations). We have modified this text (and the discussion of the choice of cutoff in the Discussion) to clarify this point. Please see revised text in response to Michel Crucifix's review.

Comment Lines 288: How does your product compare with the original Bartlein et al 2011, and the GCM-based prior? Could you show this?

Response: The GCM-based prior is shown in SI Figure 1 and the original pollen-based reconstructions (from Bartlein et al, 2011 and from Prentice et al., 2017) are shown in SI Figure 3. Comparison of these figures with the analytical reconstructions shown in the paper in Figure 4 shows the difference with our product. We could add a new set of figures to the Supplementary showing difference maps, if necessary.

Comment: How well is the seasonality captured and how does it differ from the simulated seasonality in the GCM prior?

Response: We have no independent measure of seasonality that can be used to assess the analytical reconstructions. The analytical reconstructions of MTCO and MTWA, the difference between which is the measure of the strength of temperature seasonality, are only shown when the pollen-based reconstructions contain sufficient information to modify the model-based prior and thus when the uncertainty in the pollen-based reconstructions is small. We could produce maps showing the temperature seasonality from the analytical reconstructions and the

model ensemble (and the difference between them) but these would not add anything to the manuscript beyond what is shown by the MTCO and MTWA reconstructions.

Editor's Comments

Comment: line 272: the "-" in "-5.6" should be a real minus sign.

Response: We have changed this.

Comment: Figure 4 shows climate anomalies w.r.t the CRU average for 1960-1990. This should be clearly stated in the caption.

Response:

Comment: line 859: the "e" should be in italic

Response: We have changed this

We have added a code/data availability section, author contributions and competing interests statement.

1 **A new multi-variable benchmark for Last Glacial Maximum climate simulations**

2

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5

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14

15 Journal: *Climate of the Past*

16

17 **Abstract.** We present a new global reconstruction of seasonal climates at the Last
18 Glacial Maximum (LGM, 21,000 yr BP) made using 3-D variational data assimilation
19 with pollen-based site reconstructions of six climate variables and the ensemble average
20 of the PMIP3/CMIP5 simulations as a prior. We assume that the correlation matrix of

21 the uncertainties of the prior both spatially and temporally is Gaussian, in order to
22 produce a climate reconstruction that is smoothed both from month to month and from
23 grid cell to grid cell. The pollen-based reconstructions include mean annual temperature
24 (MAT), mean temperature of the coldest month (MTCO), mean temperature of the
25 warmest month (MTWA), growing season warmth as measured by growing degree
26 days above a baseline of 5°C (GDD₅), mean annual precipitation (MAP) and a moisture
27 index (MI), which is the ratio of MAP to mean annual potential evapotranspiration.

28 Different variables are reconstructed at different sites, but our approach both preserves
29 seasonal relationships and allows a more complete set of seasonal climate variables to
30 be derived at each location. We further account for the ecophysiological effects of low
31 atmospheric carbon dioxide concentration on vegetation in making reconstructions of
32 MAP and MI. This adjustment results in the reconstruction of wetter climates than
33 might otherwise be inferred by the vegetation composition. Finally, by comparing the

34 uncertainty contribution to the final reconstruction, we provide confidence intervals on
35 these reconstructions and delimit geographical regions for which the palaeodata provide
36 no information to constrain the climate reconstructions. The new reconstructions will

37 provide a benchmark created using clear and defined mathematical procedures that can
38 be used for evaluation of the PMIP4/CMIP6 entry-card LGM simulations and are
39 available at DOI:10.17864/1947.229.

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44 1 Introduction

45 Models that perform equally well for present-day climate nevertheless produce very
46 different responses to anthropogenic forcing scenarios through the 21st century.
47 Although internal variability contributes to these differences, the largest source of
48 uncertainty in model projections in the first three to four decades of the 21st century
49 stems from differences in the response of individual models to the same forcing
50 (Kirtman et al., 2013). Thus, the evaluation of models based on modern observations is
51 not a good guide to their future performance, largely because the observations used to
52 assess model performance for present-day climate encompass too limited a range of
53 climate variability to provide a robust test of the ability to simulate climate changes.
54 Although past climate states do not provide analogues for the future, past climate
55 changes provide a unique opportunity for out-of-sample evaluation of climate model
56 performance (Harrison et al., 2015).

57

58 At the Last Glacial Maximum (LGM, [conventionally defined for modelling](#)
59 [purposes as](#) 21 000 years ago), insolation was quite similar to the present, but global
60 ice volume was at a maximum, eustatic sea level was close to a minimum, long-lived
61 greenhouse gas concentrations were lower, and atmospheric aerosol loadings higher
62 than today, and land surface characteristics (including vegetation distribution) were
63 also substantially different from today. These changes gave rise to a climate radically
64 different from that of today; indeed the magnitude of the change in radiative forcing
65 between LGM and pre-industrial climate is comparable to high-emissions projections
66 of climate change between now and the end of the 21st century (Braconnot et al., 2012).
67 The LGM has been a focus for model evaluation in the Paleoclimate Modelling
68 Intercomparison Project (PMIP) since its inception (Joussaume and Taylor, 1995;
69 Braconnot et al., 2007; Braconnot et al., 2012). The LGM is one of the two “entry card”
70 palaeoclimate simulations included in the current phase of the Coupled Model
71 Intercomparison Project (CMIP6) (Kageyama et al., 2018). The evaluation of previous
72 generations of palaeoclimate simulations has shown that the large-scale thermodynamic
73 responses seen in 21st century and LGM climates, including enhanced land–sea
74 temperature contrast, latitudinal amplification, and scaling of precipitation with
75 temperature, are likely to be realistic (Izumi et al., 2013; Li et al., 2013; Lunt et al,
76 2013; Hill et al., 2014; Izumi et al., 2014; Harrison et al., 2015). However, evaluation
77 against palaeodata shows that even when the sign of large-scale climate changes is
78 correctly predicted, the patterns of change at a regional scale are often inaccurate and
79 the magnitudes of change often underestimated (Brewer et al., 2007; Mauri et al., 2014;
80 Perez Sanz et al., 2014; Bartlein et al., 2017). The current focus on understanding what
81 causes mismatches between reconstructed and simulated climates is a primary
82 motivation for developing benchmark data sets that represent regional climate changes
83 comprehensively enough to allow a critical evaluation of model deficiencies.

84

85 Many sources of information can be used to reconstruct past climates. Pollen-based
86 reconstructions are the most widespread, and pollen-based data were the basis for the
87 current standard LGM benchmark data set by Bartlein et al. (2011). In common with
88 other data sources, the pollen-based reconstructions were generated for individual sites.
89 Geological preservation issues mean that the number of sites available inevitably
90 decreases through time (Bradley, 2014). Since pollen is only preserved for a long time
91 in anoxic sediments, the geographic distribution of potential sites is biased towards
92 climates that are relatively wet today. Furthermore, the actual sampling of potential
93 sites is highly non-uniform, so there are large geographic gaps in data coverage
94 (Harrison et al., 2016). The lack of continuous climate fields is not ideal for model
95 evaluation, and so attempts have been made to generalize the site-based data either
96 through gridding, interpolation, or some form of multiple regression (see e.g. Bartlein
97 et al., 2011; Annan and Hargreaves, 2013). ~~However, there has so far been no attempt
98 to produce a physically consistent, multi-variable reconstruction which provides the
99 associated uncertainties explicitly.~~

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100
101 A further characteristic of the LGM that creates problems for quantitative
102 reconstructions based on pollen data is the much lower atmospheric carbon dioxide
103 concentration, [CO₂], compared to the pre-industrial Holocene. [CO₂] has a direct effect
104 on plant physiological processes. Low [CO₂] as experienced by plants at the LGM is
105 expected to have led to reduced water-use efficiency – the ratio of carbon assimilation
106 to the water lost through transpiration (Bramley et al., 2013). Most reconstructions of
107 moisture variables from pollen data, including most of the reconstructions used by
108 Bartlein et al. (2011), do not take [CO₂] effects into account. Yet several modelling
109 studies have shown that the impact of low [CO₂] around the LGM on plant growth and
110 distribution was large (e.g. Jolly and Haxeltine, 1997; Cowling and Sykes, 1999;
111 Harrison and Prentice, 2003; Bragg et al., 2013; Martin Calvo et al., 2014; Martin Calvo
112 and Prentice, 2015). A few reconstructions of LGM climate based on the inversion of
113 process-based biogeography models have also shown large effects of low [CO₂] on
114 reconstructed LGM palaeoclimates (e.g. Guiot et al., 2000; Wu et al., 2007). The
115 reconstructions of moisture variables in the Bartlein et al. (2011) data set are thus
116 probably not reliable, and likely to be biased low.

117 Prentice et al. (2017) demonstrated an approach to correct reconstructions of moisture
118 variables for the effect of [CO₂], but this correction has not been applied globally. A
119 key side effect of applying this [CO₂] correction is to reconcile semi-quantitative
120 hydrological evidence for wet conditions at the LGM with the apparent dryness
121 suggested by the vegetation assemblages (Prentice et al., 2017). Similar considerations
122 apply to the interpretation of future climate changes in terms of vegetational effects.
123 Projections of future aridity (based on declining indices of moisture availability) linked
124 to warming are unrealistic, in a global perspective, because of the counteracting effect
125 of increased water use efficiency due to rising [CO₂] – which is generally taken into

129 account by process-based ecosystem models, but not by statistical models, using
130 projected changes in vapour pressure deficit or some measure of plant-available water,
131 (Keenan et al., 2011; Roderick et al., 2015; Greve et al., 2017).

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132
133 In this paper, we use variational data assimilation based on both pollen-based climate
134 reconstructions and climate model outputs to arrive at a best-estimate analytical
135 reconstruction of LGM climate, explicitly taking account of the impact of [CO₂].
136 Variational techniques provide a way of combining observations and model outputs to
137 produce climate reconstructions that are not exclusively constrained to one source of
138 information or the other (Nichols, 2010). We use the uncertainty contributions to the
139 analytical reconstruction to provide confidence intervals for these reconstructions and
140 also to delimit geographical regions for which the palaeodata provide no constraint on
141 the reconstructions. The resulting data set is expected provide a well-founded multi-
142 variable LGM climate dataset for palaeoclimate model benchmarking in CMIP6.

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145 2 Methods

146 2.1 Pollen-based climate reconstructions

147
148 Bartlein et al. (2011) provided a global synthesis of pollen-based quantitative climate
149 reconstructions for the LGM. The Bartlein et al. (2011) data set includes reconstructions
150 of climate anomalies (differences between LGM and recent climates) for six variables
151 (and their uncertainties), specifically mean annual temperature (MAT), mean
152 temperature of the coldest month (MTCO), mean temperature of the warmest month
153 (MTWA), growing degree days above a baseline of above 5°C (GDD5), mean annual
154 precipitation (MAP), and an index of plant-available moisture (the ratio of actual to
155 equilibrium evapotranspiration, or α). There are a small number of LGM sites (94) in
156 the Bartlein et al. (2011) data set where model inversion was used to make the
157 reconstructions of α and MAP; no [CO₂] correction is applied to these
158 reconstructions. There are no data from Australia in the Bartlein et al. (2011) data set,
159 and we therefore use quantitative reconstructions of MAT and another moisture index
160 (MI), the ratio of MAP to potential evapotranspiration, from Prentice et al. (2017).
161 Prentice et al. (2017) provide values of MI both before and after correction for [CO₂];
162 we use the uncorrected values in order to apply the correction for [CO₂] within our
163 assimilation framework. For consistency between the two data sets, we re-expressed
164 reconstructions of α in terms of MI via the Fu-Zhang formulation of the Budyko
165 relationship between actual evapotranspiration, potential evapotranspiration and
166 precipitation (Zhang et al., 2004; Gallego-Sala et al., 2016).

Deleted: these were excluded from our analysis

167
168 The spatial coverage of the final data set is uneven (Figure 1). There are many more
169 data points in Europe and North America than elsewhere. South America has the fewest

174 (14 sites). The number of variables available at each site varies: although most sites
175 (279) have reconstructions of at least three variables, some sites have reconstructions
176 of only one variable (60). Nevertheless, in regions where there is adequate coverage,
177 the reconstructed anomaly patterns are coherent, plausible and consistent among
178 variables.

179

180

181 For this application, we derived absolute LGM climate reconstructions by adding the
182 reconstructed climate anomalies at each site to the modern climate values from the
183 Climate Research Unit (CRU) historical climatology data set (CRU CL v2.0 dataset,
184 New et al., 2002), which provides climatological averages of monthly temperature,
185 precipitation and cloud cover fraction for the period 1961-1990 CE. Most of the climate
186 variables (MTCO, MTWA, MAT, MAP) can be calculated directly from the CRU CL
187 v2.0 dataset. GDD5 was calculated from pseudo-daily data derived by linear
188 interpolation of the monthly temperatures. MI was calculated from the CRU climate
189 variables using the radiation calculations in the SPLASH model (Davis et al., 2017).
190 For numerical efficiency, we non-dimensionalised all of the absolute climate
191 reconstructions (and their standard errors) before applying the variational techniques
192 (for details, see Cleator et al., 2019a).

193

194

195 **2.2 Climate model simulations**

196 Eight LGM climate simulations (Table 1) from the third phase of the
197 Palaeoclimate Modelling Intercomparison Project (PMIP3: Braconnot et al., 2012)
198 were used to create a prior. The PMIP LGM simulations were forced by known changes
199 in incoming solar radiation, changes in land-sea geography and the extent and location
200 of ice sheets, and a reduction in $[\text{CO}_2]$ to 185 ppm (see Braconnot et al., 2012 for details
201 of the modelling protocol). We used the last 100 years of each LGM simulation. We
202 interpolated monthly precipitation, monthly temperature and monthly fraction of
203 sunshine hours from each LGM simulation and its pre-industrial (PI) control to a
204 common $2 \times 2^\circ$ grid. Simulated climate anomalies (LGM minus PI) for each grid cell
205 were then added to modern climate values calculated from the CRU CL 2.0 data set
206 (New et al., 2002), as described for the pollen-based reconstructions, to derive absolute
207 climate values. We calculated the multi-model mean and variance (Figure 2) across the
208 models for each of the climate variables to produce the gridded map used as the prior.

209

210 **2.3 Water-use efficiency calculations**

211

212 We applied the general approach developed by Prentice et al. (2017) to correct pollen-
213 based statistical reconstructions to account for $[\text{CO}_2]$ effects. The approach as
214 implemented here is based on equations (Appendix 1) that link moisture index (MI) to

215 transpiration and the ratio of leaf-internal to ambient CO₂. The correction is based on
216 the principle that the rate of water loss per unit carbon gain is inversely related to
217 effective moisture availability as sensed by plants. The method involves solving a non-
218 linear equation that relates rate of water loss per unit carbon gain to MI, temperature
219 and CO₂ concentration. The equation is derived from theory that predicts the response
220 of the ratio of leaf-internal to ambient [CO₂] to vapour pressure deficit and temperature
221 (Prentice et al., 2014; Wang et al., 2014).

222

223 **2.4 Application of variational techniques**

224

225 Variational data assimilation techniques provide a way of combining observations
226 and model outputs to produce climate reconstructions that are not exclusively
227 constrained to one source of information or the other (Nichols, 2010). We use the
228 3D-variational method, described in Cleator et al. (2019a) to find the maximum a
229 posteriori estimate (or analytical reconstruction) of the palaeoclimate given the
230 site-based reconstructions and the model-based prior. The method constructs a
231 cost function, which describes how well a particular climate matches both the site-
232 based reconstructions and the prior, by assuming the reconstructions and prior
233 have a Gaussian distribution. To avoid sharp changes in time and/or space in the
234 analytical reconstructions, the method assumes that the prior temporal and
235 spatial covariance correlations are derived from a modified Bessel function, in
236 order to create a climate anomaly field that is smooth both from month to month
237 and from grid cell to grid cell. The degree of correlation is controlled through two
238 length scales: a spatial length scale that determines how correlated the covariance
239 in the prior is between different geographical areas, and a temporal length scale
240 that determines how correlated it is through the seasonal cycle. The site-based
241 reconstructions are assumed to have negligible correlations at these space and
242 time scales. The maximum a posteriori estimate is found by using the limited
243 memory Broyden- Fletcher-Goldfarb-Shanno method (Liu and Nocedal 1989) to
244 determine the climate that minimises the cost function. A first order estimate of
245 the analysis uncertainty covariance is also computed.

246

247 An observation operator based on calculations of the direct impact of [CO₂] on
248 water-use efficiency (section 2.3) is used in making the analytical reconstructions.
249 The prior is constructed as the average of eight LGM climate simulations (section
250 2.2). We use an ensemble of different model responses to the same forcing to
251 provide a series of physically consistent possible states, which can be viewed as
252 perturbed responses and provide the variance around the climatology provided
253 by the ensemble average. The prior uncertainty correlations are based on a
254 temporal length scale (Lt) of 1 month and a spatial length scale (Ls) of 400km.
255 Cleator et al. (2019a) have shown that a temporal length scale of 1 month

256 provides an adequately smooth solution for the seasonal cycle, both using single
257 sites and over multiple grid cells, as shown by the sensitivity of the resolution
258 matrix (Menke, 2012; Delahaies et al., 2017) to changes in the temporal length
259 scale. Consideration of the spatial spread of variance in the analytical
260 reconstruction shows that a spatial length scale of 400km also provides a
261 reasonable reflection of the large-scale coherence of regional climate change.

262
263 We generated composite variances on the analytical reconstructions (Figure 3) by
264 combining the covariances from the site-based reconstructions and from the
265 prior. There are regions where all of the models systematically differ from the site-
266 based reconstructions (Harrison et al., 2015) but nevertheless the inter-model
267 variability is low, which would lead to a very small contribution to the composite
268 uncertainties from the prior. We therefore calculated the uncertainty of the prior
269 from an equal combination of the global uncertainty, the average variance
270 between each grid cell, and local uncertainty, the variance between the different
271 models. The reliability of the analytical reconstructions was assessed by
272 comparing these composite covariances with the uncertainties in the prior. We
273 masked out cells where the inclusion of site-based reconstructions does not
274 produce an improvement of > 5% from the prior. Since this assessment is based
275 on a change in the variance, rather than absolute values, this masking removes
276 regions where there are no pollen-based reconstructions or the pollen-based
277 reconstructions have very large uncertainties.

278
279

280 3 Results

281

282 The analytical reconstructions (Figure 4) show an average year-round cooling of -5.6
283 $^{\circ}\text{C}$ in the northern extratropics. The cooling is larger in winter (-7.6°C) than in summer
284 (-2.4°C). A limited number of grid cells in central Eurasia show warmer-than-present
285 summers, and higher MAT. Temperature changes are more muted in the tropics, with
286 an average change in MAT of -3.7°C . The cooling is somewhat lower in summer than
287 winter (-2.7°C compared to -4.1°C). Reconstructed temperature changes were slightly
288 larger in the southern extratropics, with average changes in MAT of -5.0°C , largely
289 driven by cooling in winter.

290

291 Changes in moisture-related variables (MAP, MI) across the northern hemisphere are
292 geographically more heterogeneous than temperature changes. Reconstructed MAP is
293 greater than present in western North America (172 mm) but less than present (-29
294 mm) in eastern North America. Most of Europe is reconstructed as drier than present
295 (-305 mm), the same for eastern Eurasia (-94 mm) and the Far East (-66 mm). The
296 patterns in MI are not identical to those in MAP, because of the influence of temperature

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310 on MI, but regional changes are generally similar to those shown by MAP. Most of the
311 tropics are shown as drier than present while the southern hemisphere extratropics are
312 wetter than present, in terms of both MAP and MI.

313
314 The reconstructed temperature patterns are not fundamentally different from those
315 shown by Bartlein et al. (2011) but the analytical dataset provides information for a
316 much larger area (1153% increase) thanks to the method's imposition of consistency
317 among different climate variables, and smooth variations both in space and through the
318 seasonal cycle. There are systematic differences, however, between the analytical
319 reconstructions and the pollen-based reconstructions in terms of moisture-related
320 variables (MAP, MI) because the analytical reconstructions take account of the direct
321 influence of [CO₂] on plant growth. The physiological impact of [CO₂] leads to
322 analytical reconstructions indicating wetter than present conditions in many regions,
323 (Figure 5a, Figure 5b), for example in southern Africa where several of the original
324 pollen-based reconstructions show no change in MAP or MI compared to present, but
325 the analytical reconstruction shows wetter conditions than present. In some regions,
326 incorporating the impact of [CO₂] reverses the sign of the reconstructed changes. Part
327 of northern Eurasia is reconstructed as being wetter than present, despite pollen-based
328 reconstructions indicating conditions drier than present (both in terms of MAP and MI),
329 as shown by SI Figure 3. The relative changes in MAP and MI are similar across all
330 sites (Figure 5c), implying that the analytically reconstructed changes are driven by
331 changes in precipitation rather than temperature.

332

333

334 4 Discussion

335

336 Variational data assimilation techniques provide a way of combining observations and
337 model outputs, taking account the uncertainties in both, to produce a best-estimate
338 analytical reconstruction of LGM climate. These reconstructions extend the
339 information available from site-based reconstructions both spatially and through the
340 seasonal cycle. Our new analytical data set characterizes the seasonal cycle across a
341 much larger region of the globe than the data set that is currently being used for
342 benchmarking of palaeoclimate model simulations. We therefore suggest that this data
343 set (Cleator et al. 2019b) should be used for evaluating the CMIP6-PMIP4 LGM
344 simulations.

345

346 Some areas are still poorly covered by quantitative pollen-based reconstructions of
347 LGM climate, most notably South America. More pollen-based climate reconstructions
348 would provide one solution to this problem – and there are many pollen records that
349 could be used for this purpose (Flantua et al., 2015; Herbert and Harrison, 2016;
350 Harrison et al., 2016). There are also quantitative reconstructions of climate available
351 from individual sites (e.g. Lebamba et al., 2012; Wang et al., 2014; Loomis et al., 2017;

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Deleted: , and this largely reflects the influence of [CO₂] that is included in the analysis.

Deleted: Accounting for the physiological impact of [CO₂] means that the analytical reconstructions indicate wetter than present conditions in many regions

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360 [Camuera et al., 2019](#)) that should be incorporated into future data syntheses. It would
361 also be possible to incorporate other sources of quantitative information, such as
362 [chironomid-based reconstructions \(e.g. Chang et al., 2015\)](#), within the variational data
363 assimilation framework.

364

365 One of the benefits of the analytical framework applied here is that it allows the
366 influence of changes in [CO₂] on the moisture reconstructions to be taken into account.
367 Low [CO₂] must have reduced plant water-use efficiency, because at low [CO₂] plants
368 need to keep stomata open for longer in order to capture sufficient CO₂. [Statistical
369 reconstruction methods that use modern relationships between pollen assemblages and
370 climate under modern conditions \(i.e. modern analogues, transfer functions, response
371 surfaces: see Bartlein et al., 2011 for discussion\) cannot account for such effects.](#)

372 Climate reconstruction methods based on the inversion of process-based ecosystem
373 models can do so (see e.g. Guiot et al., 2000; Wu et al., 2007; Wu et al., 2009; Izumi
374 and Bartlein, 2016) but are critically dependent on the reliability of the vegetation
375 model used. Most of the palaeoclimate reconstructions have been made by inverting
376 some version of the BIOME model (Kaplan et al., 2003), which makes use of
377 bioclimatic thresholds to separate different plant functional types (PFTs). As a result,
378 reconstructions made by inversion show “jumps” linked to shifts between vegetation
379 types dominated by different PFTs whereas, as has been shown recently (Wang et al.,
380 2017), differences in water use efficiency of different PFTs can be almost entirely
381 accounted for by a single equation, as proposed here. [Sensitivity analyses show that the
382 numerical value of the corrected moisture variables \(MI, MAP\) is dependent on the
383 reconstructed values of these variables but is insensitive to uncertainties in the
384 temperature and moisture inputs \(Prentice et al., 2017\). The strength of the correction
385 is primarily sensitive to \[CO₂\], but the LGM \[CO₂\] value is well constrained from ice-
386 core records.](#) The response of plants to changes in [CO₂] is non-linear (Harrison and
387 Bartlein, 2012), and the effect of the change between recent and pre-industrial or mid-
388 Holocene conditions is less than that between pre-industrial and glacial conditions.
389 [Nevertheless, it would be worth taking the \[CO₂\] effect on water-use efficiency into
390 account in making reconstructions of interglacial time periods as well.](#)

391

392 The influence of individual pollen-based reconstructions on the analytical
393 reconstruction of seasonal variability, or the geographic area influenced by an
394 individual site, is crucially dependent on the choice of length scales. We have adopted
395 conservative length scales of 1 month and 400 km, based on sensitivity experiments
396 made for southern Europe (Cleator et al., 2019a). These length scales produce
397 numerically stable results for the LGM, and the paucity of data for many regions at the
398 LGM means that using fixed, conservative length scales is likely to be the only practical
399 approach. However, in so far as the spatial length scale is related to atmospheric
400 circulation patterns, there is no reason to suppose that the optimal spatial length scale
401 will be the same from region to region. The density and clustering of pollen-based

Deleted: Statistical reconstruction methods, whether based on modern analogues or modern climate transfer functions, cannot account for such effects.

Deleted: Nevertheless, it would be worth taking this effect into account in making reconstructions of interglacial time periods as well.

408 reconstructions could also have a substantial effect on the optimal spatial length scale.
409 A fixed 1-month temporal length scale is appropriate for climates that have a reasonably
410 smooth and well-defined seasonal cycle, either in temperature or precipitation.
411 However, in climates where the seasonal cycle is less well defined, for example in the
412 wet tropics, or in situations where there is considerable variability on sub-monthly time
413 scales, other choices might be more appropriate. For time periods such as the mid-
414 Holocene, which have an order of magnitude more site-based data, it could be useful to
415 explore the possibilities of variable length scales.

416

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

430

431 There have been a few previous attempts to use data assimilation techniques to generate
432 spatially continuous palaeoclimate reconstructions. Annan and Hargreaves (2013) used
433 a similar multi-model ensemble as the prior and the pollen-based reconstructions from
434 Bartlein et al. (2011) to reconstruct MAT at the LGM. However, they made no attempt
435 to reconstruct other seasonal variables, either independently, or through exploiting
436 features of the simulations (as we have done here) to generate seasonal reconstructions.
437 Particle filter approaches (e.g. Goosse et al., 2006; Dubinkina et al., 2011) produce
438 dynamic estimates of palaeoclimate, but particle filters cannot produce estimates of
439 climate outside the realm of the model simulations. Our 3-D variational data
440 assimilation approach has the great merit of being able to produce seasonally coherent
441 reconstructions generalized over space, while at the same time being capable of
442 producing reconstructions that are outside those captured by the climate model, because
443 they are not constrained by a specific source (Nichols, 2010). This property is of
444 particular importance if the resulting data set is to be used for climate model evaluation,
445 as we propose.

446

447 Data availability. The gridded data for the LGM reconstructions are available
448 from DOI:10.17864/1947.229; the code used to generate these reconstructions is
449 available from DOI:10.5281/zenodo.3445166.

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Deleted: Kalman particle filter approaches (e.g. Goosse et al., 2006) produce seasonal and geographical estimates of palaeoclimate, but particle filters cannot produce estimates of climate outside the realm of the model simulations.

455 **Author Contributions**

456 All authors contributed to the design of the study; ICP developed the theory
457 underlying the CO₂ correction; SC implemented the analyses. SC and SPH wrote
458 the first version of the manuscript, and all authors contributed to the final version.

460 **Competing Interests.**

461 The authors declare they have no competing interests.

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779 **Figures and Tables Captions**

780

781 Figure 1: The distribution of the site-based reconstructions of climatic variables at the
782 Last Glacial Maximum. The individual plots show sites providing reconstructions of
783 (a) moisture index (MI), (b) mean annual precipitation (MAP), (c) mean annual
784 temperature (MAT), (d) mean temperature of the coldest month (MTCO), (e) mean
785 temperature of the warmest month (MTWA) and growing degree days above a baseline
786 of 5° C (GDD5). The original reconstructions are from Bartlein et al. (2011) and
787 Prentice et al. (2017).

788

789 Figure 2: Uncertainties associated with the climate prior. The climate is derived from a
790 multi-model mean of the ensemble of models from the Palaeoclimate Modelling
791 Intercomparison Project (PMIP) and is shown in SI Figure 1. The uncertainties shown
792 here are the standard deviation of the multi-model ensemble values. The individual
793 plots show the variance for the simulated (a) moisture index (MI), (b) mean annual
794 precipitation (MAP), (c) mean annual temperature (MAT), (d) mean temperature of the
795 coldest month (MTCO), (e) mean temperature of the warmest month (MTWA) and
796 growing degree days above a baseline of 5° C (GDD5).

797

798 Figure 3: Uncertainties on the analytical reconstructions. These uncertainties
799 represent a combination of the uncertainty on the site-based reconstructions, and
800 the grid-based variance on the prior and the global variance from the prior.

801

802 Figure 4: Analytically reconstructed climate, where areas for which the site-based data
803 provide no constraint on the prior have been masked out. The individual plots show
804 reconstructed (a) moisture index (MI), (b) mean annual precipitation (MAP), (c) mean
805 annual temperature (MAT), (d) mean temperature of the coldest month (MTCO), (e)
806 mean temperature of the warmest month (MTWA) and growing degree days above a
807 baseline of 5° C (GDD5). The anomalies are expressed relative to the long term average
808 (1960-1990) values from the Climate Research Unit (CRU) historical climatology data
809 set (CRU CL v2.0 dataset, New et al., 2002).

810

811

812 Figure 5: Impact of CO₂ on reconstructions of moisture-related variables. The
813 individual plots show (a) the change in moisture index (MI) and (b) the change in mean
814 annual precipitation (MAP) compared to the original pollen-based reconstructions for
815 the LGM before (circles) and after (crosses) the physiological impacts of [CO₂] on
816 water-use efficiency are taken into account. The third plot (c) shows the relative
817 difference in MI and MAP as a result of [CO₂], shown as the percentage difference
818 between the no-[CO₂] and [CO₂] calculations.

819

Deleted: uncertainties

Deleted: These uncertainties represent a combination of the errors on the site-based reconstructions, and the grid-based errors on the prior and the global uncertainty from the prior.

Deleted: 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) 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.

832 Table 1: Details of the models from the Palaeoclimate Modelling Intercomparison
 833 Project (PMIP) that were used for the Last Glacial Maximum (LGM) simulations used
 834 to create the prior.

835

836 *Table 1: Details of the models from the third phase of the Palaeoclimate Modelling*
 837 *Intercomparison Project (PMIP3) that were used for the Last Glacial Maximum*
 838 *(LGM) simulations used to create the prior. Coupled ocean-atmosphere models are*
 839 *indicated as OA, which OAC models have a fully interactive carbon cycle. The*
 840 *resolution in the atmospheric, oceanic and sea ice components of the models is given*
 841 *in terms of numbers of grid cells in latitude and longitude.*

842

Model name	Type	Resolution			Year length	Reference
		Atmosphere	Ocean	Sea Ice		
CCSM4	OA	192, 288	320, 384	320, 384	365	Gent et al. (2011)
CNRM-CM5	OA	128, 256	292, 362	292, 362	365-366	Voldoire et al. (2012)
MPI-ESM-P	OA	96, 192	220, 256	220, 256	365-366	Jungclaus et al. (2006)
MRI-CGCM3	OA	160, 320	360, 368	360, 368	365	Yukimoto et al. (2011)
FGOALS-g2	OA	64, 128	64, 128	64, 128	365	Li et al. (2013)
COSMOS-ASO	OAC	96, 48	120, 101	120, 101	360	Budich et al. (2010)
IPSL-CM5A-LR	OAC	96, 96	149, 182	149, 182	365	Dufresne et al., 2013
MIROC-ESM	OAC	64, 128	192, 256	192, 256	365	Watanabe et al. (2011)

843

844 Appendix

845 We define e as the water lost by transpiration (E) per unit carbon gained by
846 photosynthesis (A). This term, the inverse of the water use efficiency, is given by:

$$847 \quad e = E/A = 1.6 D / ((1 - \chi) c_a) \quad (\text{A1})$$

848 where D is the leaf-to-air vapour pressure deficit (Pa), c_a is the ambient CO₂ partial
849 pressure (Pa) and χ is the ratio of leaf-internal CO₂ partial pressure (c_i) to c_a . An
850 optimality-based model (Prentice *et al.* 2014), which accurately reproduces global
851 patterns of χ and its environmental dependencies inferred from leaf $\delta^{13}\text{C}$ measurements
852 (Wang *et al.* 2017), predicts that:

$$853 \quad \chi = (\Gamma^*/c_a) + (1 - \Gamma^*/c_a) \xi / (\xi + \sqrt{D}) \quad (\text{A2a})$$

854 and

$$855 \quad \xi = \sqrt{(\beta(K + \Gamma^*)/1.6 \eta^*)} \quad (\text{A2b})$$

856 where Γ^* is the photorespiratory compensation point of C₃ photosynthesis (Pa), β is a
857 constant (estimated as 240 by Wang *et al.* 2017), K is the effective Michaelis-Menten
858 coefficient of Rubisco (Pa), and η^* is the ratio of the viscosity of water (Pa s) at ambient
859 temperature to its value at 25°C. Here K depends on the Michaelis-Menten coefficients
860 of Rubisco for carboxylation (K_C) and oxygenation (K_O), and on the partial pressure of
861 oxygen O (Farquhar *et al.* 1980):

$$862 \quad K = K_C (1 + O/K_O) \quad (\text{A3})$$

863 Standard values and temperature dependencies of K_C , K_O , Γ^* and η^* are assigned as in
864 Wang *et al.* (2017).

865 The moisture index MI is expressed as

$$866 \quad \text{MI} = P/E_q, E_q = \sum_n (R_n/\lambda) s/(s + \gamma) \quad (\text{A4})$$

867 where P is annual precipitation, R_n is net radiation for month n , λ is the latent heat of
868 vaporization of water, s is the derivative of the saturated vapour pressure of water with
869 respect to temperature (obtained from a standard empirical formula also used by Wang
870 *et al.* 2017), and γ is the psychrometer constant. We assume that values of MI
871 reconstructed from fossil pollen assemblages, using contemporary pollen and climate
872 data either in a statistical calibration method or in a modern-analogue search, need to
873 be corrected in such a way as to preserve the contemporary relationship between MI
874 and e , while taking into account the change in e that is caused by varying c_a and
875 temperature away from contemporary values. The sequence of calculations is as
876 follows. (1) Estimate e and its derivative with respect to temperature ($\partial e/\partial T$) for the
877 contemporary c_a and climate, using equations (A1) – (A3) above. (2) Use the e and
878 $\partial e/\partial T$ to calculate $\partial D/\partial T$ given the palaeo c_a (measured in ice-core data) and
879 temperature (reconstructed from pollen data), via a series of analytical equations that
880 relate $\partial e/\partial T$ to $\partial D/\partial T$ and hence to s . (3) Use the new $\partial D/\partial T$ and relative humidity (from
881 the PMIP3 average) to derive a new value of s . (4) Re-calculate MI using a palaeo
882 estimate of R_n (modelled as in Davis *et al.*, 2017) and the new value of s .

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