

August 1, 2019

Helen McGregor  
Editor, *Climate of the Past*

Dear Dr. McGregor:

We are pleased to resubmit our revised manuscript introducing the Joint Proxy Inversion method. We have addressed all reviewer comments in our manuscript and in the response text which follows this letter. Although none of the major findings, and few of the minor details of our results have changed, these updates have made the manuscript a much stronger contribution, and we thank you and the reviewers for their time and input.

The most substantial change is the use of a continuous-time formulation of the paleoenvironmental time series models, as suggested by reviewer 1. This has eliminated the need to adopt the (granted somewhat arbitrary) block interpolation method used to forward-model the proxy data in our initial submission, and makes the method more flexible overall. This all comes at the expense of increased computation time, and as we noted above produced no detectable changes in the fundamental results or interpretation of the records. However, we have updated the manuscript to present this formulation since it does in a fundamental sense represent an improvement over our previous approach.

As requested, we have released our GitHub repository through Zenodo, and now include a DOI pointing to this release as a persistent archive of the code and data.

Beyond that, additional details, clarification of the presentation and discussion, and a new supplementary figure showing the proxy calibration data and model posterior have been included. We have checked over the manuscript and materials, and hope that you agree that the contribution is now acceptable and ready for publication in *CoP*.

Sincerely,



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Reviewer comments are shown here in plain text, our initial responses in italics, and the final response/revision in bold italics.

-Reviewer 1-

A Bayesian Hierarchical Model is used to reconstruct several environmental variables using some proxy variables, at three marine sites. The method isn't new e.g. Garreta et al. (2010), but the manuscript is useful as another example of this type of approach. The manuscript is unclear in places.

*We're glad the reviewer finds value in the paper. As acknowledged in the text and citations the approach here is not without precedent. We'll add the Garreta example, another interesting one using a much more complex (dynamic vegetation) process model to our reference list in the revision.*

***We now cite the Garreta paper as an example of previous applications in the introduction.***

In S2.3 (Section 2.3) Eq. 5 is a stationary discrete-time first-order autoregression (AR1) model for the random walk disturbances  $eY$ . According to S2.3, for BWT and d18Osw this AR1 model is run at a time step of 50 kyr (site 806) and 1 kyr (site 1123 and U1385). For Mg=Casw, the manuscript states "1 Myr time steps from 80 Ma to present", but what about for the higher-resolution sites (for Mg/Casw)? Also it is not clear what happens when the model time steps are different from the marine proxy time steps (which are irregular, S2.1 paragraph 2) - this point needs to be clarified. It would be good to have a graphical depiction of the method (e.g. included in Fig. 1), with example time series (with clear time points) showing  $eY$ ,  $Y$ , modelled proxy time series e.g. d18Of, and observed time series. Just show a portion of the time series, so that the time points for each time series are clear. # Further, instead of a discrete-time model, why not use a continuous-time model, which handles irregular time steps better than a discrete-time model. For example, a continuous-time time AR1 model is: (equation) For a continuous-time AR model, the parameters are not a function of the sampling intensity (Tomasson, 2015).

*We thank the reviewer for this suggestion, and in preparing our revision will explore the idea of using a continuous-time AR1 model. This would have clear benefits (including eliminating the need for interpolation, discussed below) and assuming it is feasible for the study systems we'll intended to adopt this tweak in the revision. We do not anticipate that the change will have a strong (or maybe even detectable) impact on the key outcomes. We will also work with the reviewer's idea of illustrating the time-series model properties through an addition to figure 1, which we like in theory and will do our best to implement without compromising the clarity/focus of the figure.*

***All simulations now use a continuous-time AR1 formulation, as suggested. This produces no material change in the results obtained, but does allow more robust treatment of irregularly spaced proxy time series (previously we used block interpolation to estimate values at proxy observation points). We note as an aside that using the continuous form does increase analysis time substantially as a result of the larger number of time steps to be evaluated, so our original block interpolation scheme might be preferable in some cases.***

***We have also added a visualization of the model framework to figure 1.***

S2.4 paragraph 3: "we conducted three different analyses ... the third inverting both records together." It's not clear what is meant by the latter phrase. An example of a discrete-time vector correlated random walk model is: (equation) ... Exactly what model was used in "inverting both records

together", together with an explanation of why it would be mathematically different from "inverting data from each site independently" needs to be included in the manuscript text. Further there are vector continuous-time series models, which might be better to use for inverting multiple time series with irregular time intervals.

*The presentation here is somewhat ambiguous, and will resolve this in the revision. Our analysis remains agnostic of the correlation structure between the paleoenvironmental state variables at the two sites. They are modeled as independent time series, with no correlation term. We recognize that alternative models, such as that proposed by the reviewer, would allow incorporation of additional prior information and perhaps provide stronger process model constraints on the paleoenvironmental time series, acknowledging that they are likely not truly independent. However, the model proposed by the reviewer is just one step along a continuum of model forms that one could apply which would, at its end point, lead to a climate system model that expressed a full set of physics-based expectations for the relationship between the environmental state variables at the sites. While we acknowledge the potential value in such an analysis (which would basically become a data assimilation analysis), we are proposing and exploring a framework that lies at the other end of the continuum. Our goal is to offer a widely applicable and approachable framework in which practitioners who already routinely develop quantitative interpretations of their data without reference to any formal statistical framework or paleoenvironmental model can begin to adopt such without compromising the data-driven nature of their interpretations or having to frame them in the context of the complexity and structural assumptions of more complex paleoenvironmental models.*

***We now elaborate the form of this model and provide a few lines of context in the paragraph referenced by the reviewer.***

S3.2 paragraph 1: In statistics, the idea of smoothing (whether by frequentist or bayesian methods) stems from the idea that a time series = state variable + noise. Looking at Lear et al. (2015), the L15 reconstruction appears to have a higher variability simply because there was no smoothing employed. A better comparison here would be to create a reconstruction using both frequentist smoothing and bayesian smoothing methods, and then compare. The current comparison here seems a bit apples and oranges.

*Indeed, the crux of this comparison is smoothing, and based on the reviewer's feedback we propose to emphasize this more clearly with revisions to the language in this part of the discussion. We prefer not to present this as a comparison of Bayesian and frequentist smoothing techniques, however. The crux of our paper is not to enter into the Bayesian vs. frequentist discussion. Instead, we are trying to present an alternative to the reconstruction methods used nearly ubiquitously in the (pre-Holocene paleoclimate) community (and honestly most Holocene work), which do not embrace or consider concepts such as smoothing, multi-variate proxy models, or temporal autocorrelation of environmental timeseries. Our point in this section is that 1) smoothed reconstructions are a more realistic/honest expression of the information contained in proxy timeseries records, and that 2) the method demonstrated here offers an approach to optimize the properties of the smoothed reconstruction based on the data, rather than adopting an ad hoc approach (e.g., splines or running averages with arbitrarily specified parameters) as is commonly done if and when smoothing is conducted. The comparison is apples to oranges, but we think also of value.*

***We have edited these paragraphs to better emphasize the concept of smoothing as relevant here and note that other approaches to smoothing have and can be used.***

S3.2 paragraph 3: So if d18Osw and BWT are generated at 1 kyr time steps, and the sampling resolution of d18Of is between 1 per 110 and 1 per 1700 years, do you generate the model time series first, at 1 ka steps, and then use Eq. 5 to “integrate” to the proxy time points (if necessary)? How is that integration done?

*In our original analysis, values for proxy time points are obtained using a ‘nearest neighbor’ approach, i.e. the value at the nearest proxy time series point is used. We will clarify and discuss/justify this in the revision if we end up maintaining a discrete time series model approach, or if we adopt the continuous AR1 model this will become a moot point.*

***This issue is now moot as a continuous-time AR model is used to estimate at each proxy time point.***

S3.2 paragraph 4: The following sentence could be worded better: “Moreover, because temporal autocorrelation of the environmental variables is considered ...”. I think you are trying to say its both the autocorrelation (in the environmental states) and sample density which make the credible intervals what they are. In the next sentence, can you explain mathematically what is meant by “the strength of the proxy constraints”?

*Yes, we can work on rewording/elaborating to clarify as requested.*

***This text has been re-written to clarify the point raised in the reviewer comment.***

S3.3 paragraph 2 (“These refinements reflect ...”) After 800 ka, perhaps the higher proxy model variance is suggesting the environmental model is missing something? For example, what would be the effect of adding a stochastic periodic component to the process model to capture the 100 ka cycle after 800 ka?

*Absolutely, this conclusion is essentially what we were suggesting here. Adapting the process model would be a good, perhaps more appropriate, alternative to adapting the data model across the 800 kya boundary, and we propose to explore this alternative in preparing our revision. This will depend a bit on whether the sampling resolution of the site 806 data is adequate to constrain the sub-100 kyr variability in this interval, in which case it makes sense to treat it as ‘signal’ (i.e. in the process model) or ‘noise’ (i.e. as done, in the error term of the data model).*

***We experimented with this a bit but given that our analysis of this dataset focuses on Myr-scale trends we have opted to retain the simpler time series model parameterization in the revised manuscript. We now explain the rationale for this decision in the methods (S2.2), however, and note that using a more complex environmental model is an alternative that would be preferable under some other circumstances.***

S3.3 paragraph 3 The phrase “double-count uncertainty associated with correlated parameters” is not an elegant mathematical explanation.

*With all respect, and acknowledging the suggestion, we are not writing this for mathematicians but rather for paleoclimate practitioners. Here we are attempting to provide a common-language explanation of some of the contrasts between the proposed approach and common practice. This phrase may be somewhat imprecise, but we think it makes the point in a way that most readers will grasp it.*

***We have changed the language here and now use the more technical term “inflate”.***

It's unclear exactly how the dotted blue line in Fig. 8a is calculated. Explain. Also statistical tests don't always need to assume independence, because there are ways of accounting for autocorrelation in a statistical test.

“The net result in this case ... some 100-200 kyr earlier using the traditional approach”: would this sentence be true if autocorrelation was taken into account in the traditional approach. I'm looking for a fair comparison here.

Also for the solid blue line in Fig 8a - give details of its calculation.

*We will happily elaborate/be more specific on the calculation of the ‘traditional’ analyses presented in the figure. In the original draft we had erred on the side of brevity in an attempt to interrupt the flow during the latter part of the manuscript. We see how this compromises the clarity of the analysis, however, and will revise to ensure the calculations are described in enough detail to be reproducible from the text alone (i.e. not requiring reference to the data analysis code, which is already publically available and fully documents the details). With respect to autocorrelation – indeed this is the crux of the difference noted in figure 8a. We will try to make this clearer/provide greater emphasis in the revision. Akin to the comment above on smoothing, our point here is that the JPI framework integrates explicit treatment of time series autocorrelation, ensuring that data interpretations developed from the method reflect a robust consideration of such, unlike many analyses presented in the literature. There are other ways of achieving this, of course, and we’ll be sure to better make that point in our revision.*

***We have added the details of how each metric of change is calculated to the figure 8 caption. We have also reframed the discussion of the first comparison (Fig. 8a) to provide examples of how such analyses have been accomplished previously, emphasize the value of integrating the estimation of autocorrelation within the JPI analysis, and focus more on what learned from internal comparison rather than benchmarking against a ‘traditional’ method external to our work.***

p4 L13: “sampling resolution between 1 per 110 and 1 per 1700” years. Clarify for d18O, Mg/Ca, or both?

*This summarizes across both proxies, and we will clarify in the revised text.*

***Done***

p5 L11-12: The Evans et al. (2013) terminology includes “sensor models”, “archive models”, and “observation models”. Clarify which of your equations relate to which type of Evans's models?

*I personally have struggled with this, as I don’t think there is a 1:1 mapping in this case. Part of the issue is that the Evans et al conception includes a strong focus on the processes that integrate proxy responses in a biological or sedimentary medium that accumulates over time (e.g., sediment stack, incremental growth structure; archive model) and how those integration processes are sampled (observation model). These are not explicitly treated here, or in many proxy interpretations, and in some lower-resolution deep time studies may be less critical than in much of the higher-resolution shallow-time work (I’ll note, however, that I’m not sure I actually believe this...it is a frontier area*

*and there are now a handful of really interesting avenues being pursued, e.g., with respect to processes such as seasonal sampling of different proxy archives and the impact of sedimentary architecture and allogenic processes on signal integration/preservation). At any rate, what we have here, in my interpretation, is primarily a sensor model, which also embeds some aspect of what would appear in archive and observations models in the proxy model error term. We will state this (more concisely that I have here!) in the revision.*

***We have expanded this sentence to elaborate how the other component models of Evans et al. map to our equations.***

p5 L17: “age estimate and uncertainty” Ambiguous wording, because as is it reads “age estimate and age uncertainty”.

*We will reword as suggested.*

***Wording has been changed to eliminate ambiguity.***

Eq. 2 and 3: For clarity, can you make all the “functions” with round brackets e.g.  $BWT(tMgCaf[i])$ . Change the outer brackets too i.e.  $\{ \}$ . Keep square brackets for distributions e.g.  $N[ ]$ , as you have done.

*We will reformat the equations as suggested.*

***Done.***

Eq. 5 Say what Y can be e.g.  $Y(t)$  can be  $MgCasw(t)$  or  $d18Osw(t)$  or  $BWT(t)$ .

*We will elaborate as suggested.*

***Done.***

p8 L2: Clarify the phrase “stiff” time series behaviour (give a reference if possible)

*We will do some literature research to see if we can come up with a more formal way to express this result...we were trying here to colloquially express the condition in which error variance is small and error autocorrelation large, as for the  $Mg/Ca_{sw}$ , which leads to long burn-in times using most methods for generating MCMC step proposals.*

***Upon further investigation, we have removed this extraneous ‘common-language’ term from the description of the  $Mg/Ca_{sw}$  time series.***

p12 L8: “Across all scales”: Across all sites?

*We intended ‘across all timescales’, but the suggested ‘across all sites’ would probably be clearer and will be adopted in the revision.*

***Done.***

Additional figures showing the calibration datasets, with individual draws from the posterior distribution, should be included. These could go in the manuscript or supplementary material.

*We can easily add these to the SI in the revision, and are happy to do so.*

***New figure S4 shows examples of the calibration relationships as requested.***

Fig. 5: Which inversion did these distributions come from e.g. site 806? (include in caption)

Fig 6: same comment as Fig. 5.

*We will clarify that these are from the 806 analysis and also indicate the taxon to which they apply in the revised figure legends.*

***We have added this information to the figure captions.***

Fig. 7: The prior distributions in (d) and (g) don't integrate to 1.0 e.g.  $2.5 \times 0.8 = 2.0$ . I can't tell if all the other distributions integrate to one or not.

*Thanks for catching this...it is a plotting error (we carried over the y-axis value of 2.5 appropriate to the prior in panel a) which we will correct in the revision.*

***This error has been fixed.***

Figure 9: There is a positive relationship between DBWT and Dd18Osw in the two Miocene states (mentioned in the last sentence in S3.4). I think adding some straight lines to mark this, and not inverting the y-axis here would help the reader.

*We will certainly un-invert the y axis as suggested (appropriate here since we are plotting d18O of seawater and not carbonate). We will also explore ways of adding lines that represent the correlation in posterior values from different states.*

***We have flipped the y-axis. We have not added lines showing the positive DBWT/Dd18Osw correlation during the two Miocene states since this feature is only weakly expressed in the revised analysis.***

-Reviewer 2-

Parts of the methods section were difficult to assess because of missing references.

*We assume that the following questions point to specific cases where additional citation would be helpful, and address how and where this will be resolved in our responses below.*

***See below***

Did the authors develop proxy system models described in equations 2 and 3 or are these described elsewhere?

*These equations represent ‘standard’ widely-used forms used to describe the temperature sensitivity of foraminiferal calcite Mg/Ca and  $\delta^{18}\text{O}$  values in the literature. In our revision we will make this clear and cite some of the literature in which these forms have been previously proposed and used. We believe this will also help address some of the reviewer’s later questions about the rationale for including some of the terms in these proxy model equations (we’re adopting/testing equation forms based on precedent in the community).*

***We have elaborated and provided references in this section describing the precedent for these equations.***

Page 4 line 30: How were these uncertainties determined?

*These are approximations derived from the original data sources, we will clarify this point and add citations in the revision.*

***We have reworded this section to clarify the source of the (ballpark) uncertainty estimates.***

Page 5 line 27: How is paleo-seawater Mg/Ca determined?

*The value given here in the text here are simply first-pass estimates used in developing the priors on the foram proxy model parameters. For the non-modern (Paleocene-Eocene) samples we use a value of 1.5 mol/mol based on prior work of Lear et al. (2015). We will clarify this and add the citation to this sentence in the revision.*

***We now cite the source of this estimate in the referenced sentence.***

Page 4 line 30: How were bottom water temperature (BWT) uncertainties estimated?

*Answered above.*

***See above.***

As far as I understood page 5 lines 25 – 32, proxy system model parameters are estimated based on observed (and inferred) BWT, surface water Mg/Ca and Mg/Ca of foraminifera. The posterior distributions of these parameters are then used as prior distributions when past surface water Mg/Ca and BWT are reconstructed.

*This is almost but not quite correct. In our framework, posterior distributions for all parameters (including the proxy model parameters and the paleoenvironmental parameters) are found together. In other words, rather than first estimating the posterior of the proxy model parameters, then applying them to estimate the posterior distributions of the paleoenvironmental (process) model parameters, we simulate both sets together. To envision one implication, imagine that the ‘true’ value of one of the proxy model parameters (let’s say temperature sensitivity of foraminiferal Mg/Ca) was actually a bit higher than the average estimate. Given that, the most likely paleo-environmental temperature time series would be shifted relative to the ‘mean’ estimate, also. By solving the full system simultaneously the joint distribution of posterior parameters captures these trade-offs and can be analyzed in new ways (e.g., see some of the derived analyses later in the paper).*



***We have added a statement to this section clarifying that the initial regressions are used to develop prior distributions for the proxy model parameters.***

The authors assume a paleo-seawater Mg/Ca of 1.5 when calibrating proxy system models. How do the authors get this value and how uncertain is it? How would including uncertainties affect parameter estimates?

*As mentioned above, this value was only used in estimating the prior distribution for the Mg/Ca model parameters (and only for one species). The parameter values contained in the posterior distribution are the result of MCMC sampling of the entire model system. We have replicated the analysis using a variety of prior assumptions for the foraminiferal Mg/Ca proxy model and find little sensitivity in the posterior distributions (not shown). We will try to make this logic clearer in the revision.*

***Although we don't present a formal analysis of the impact of this assumption in the manuscript, our other results (e.g., figures 2 and 5) show that 1) the Mg/Ca value used in the estimation of proxy model priors is similar to that inferred in the full JPI analysis and should not bias the result, and 2) the priors we obtained in this way are consistent with the posterior estimates from the full inversion despite the fact that the full JPI provides additional constraints on these parameters...in other words there is a strong suggestion here (figure 5) that the prior is not strongly affecting the results obtained in the full analysis.***

Page 4: lines 28 and 29: some BWT values for calibration are based on  $\delta^{18}\text{O}$  thermometry. Please explain this method (and add references). Is  $\delta^{18}\text{O}$  thermometry based on eq 3? If yes, how were surface water  $\delta^{18}\text{O}$  values determined and how do these values influence surface water  $\delta^{18}\text{O}$  values reconstructed in this study?

*These values were only used for calibrations including data from the early Paleogene, when the globe was essentially ice-free. The BWT estimates are thus based on 'standard' assumptions for the  $\delta^{18}\text{O}$  of the ice-free ocean. The actual values used are from Lear et al. (2015), and we will add this citation to the sentence for clarity.*

***The text states the ice-free assumption and now cites the source of the estimates.***

Equation 2: Mg/Ca of foraminifera is modeled as a function of BWT and surface water Mg/Ca. However, credible intervals of  $\alpha_3$  clearly include 0 indicative of weak (or absent) influence of surface water Mg/Ca on Mg/Ca of foraminifera, which might explain the results described page 8 line 5 (proxy data doesn't seem to inform this parameter either Fig 5c). Why is surface water Mg/Ca included in this proxy model given that it doesn't have a clear influence on Mg/Ca of foraminifera?

# Equation 3:  $\delta^{18}\text{O}$  of foraminifera is modeled as a function of  $\delta^{18}\text{O}$  of surface water, BWT and  $\text{BWT}^2$ . However, credible intervals of  $\beta_3$  (parameter relating  $\text{BWT}^2$  and  $\delta^{18}\text{O}$ ) include 0 for *Cibicides* as well as *Uvigerina*. Including  $\text{BWT}^2$  in the model therefore needs additional justification. As the authors note in the discussion, posterior distributions of  $\beta_3$  place even more weight on values close to 0 than the prior distribution.

*In both cases our approach was to adopt the model forms commonly in current use within the paleoclimate community (ref. our response to the earlier question). These forms have been adopted, usually based on empirical relationships rather than fundamental considerations, and widely used in previous studies, and we chose them for consistency and comparability with prior work. However, as*

*noted by the reviewer, in some cases the results of our analysis suggest that one or more model parameters are not or only weakly informative. This result has been noted before in studies that have used traditional statistical approaches to calibrate model equations for these systems. The sensitivity to these parameters seems to vary among species, however, so that in most studies the full form of the equations (all terms) are considered so that the same form can be used for all species. Although we propose to continue to use the 'canonical' forms in our revision, we will better emphasize and elaborate on the result that our analyses do not support sensitivity to some of these model terms, which may 1) suggest that, for these species, a simpler proxy model is appropriate, and 2) slightly inflate uncertainty estimates when these terms are included.*

***We have added a statement in the discussion noting the lack of sensitivity to these parameters and indicating why we retain them in our analysis.***

# Joint inversion of proxy system models to reconstruct paleoenvironmental time series from heterogeneous data

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**Abstract.** Paleoclimatic and paleoenvironmental reconstructions are fundamentally uncertain because no proxy is a direct record of a single environmental variable of interest; all proxies are indirect and sensitive to multiple forcing factors. One productive approach to reducing proxy uncertainty is the integration of information from multiple proxy systems with complimentary, overlapping sensitivity. Most such analyses are conducted in an ad-hoc fashion, either through qualitative comparison to assess the similarity of single-proxy reconstructions or through step-wise quantitative interpretations where one proxy is used to constrain a variable relevant to the interpretation of a second proxy. Here we propose the integration of multiple proxies via the joint inversion of proxy system and paleoenvironmental time series models in a Bayesian hierarchical framework. The “Joint Proxy Inversion” (JPI) method provides a statistically robust approach to producing self-consistent interpretations of multi-proxy datasets, allowing full and simultaneous assessment of all proxy and model uncertainties to obtain quantitative estimates of past environmental conditions. Other benefits of the method include the ability to use independent information on climate and environmental systems to inform the interpretation of proxy data, to fully leverage information from unevenly- and differently-sampled proxy records, and to obtain refined estimates of proxy model parameters that are conditioned on paleo-archive data. Application of JPI to the marine Mg/Ca and  $\delta^{18}\text{O}$  proxy systems at two distinct timescales demonstrates many of the key properties, benefits, and sensitivities of the method, and produces new, statistically-grounded reconstructions of Neogene ocean temperature and chemistry from previously published data. We suggest that JPI is a universally applicable method that can be implemented using proxy models of wide-ranging complexity to generate more robust, quantitative understanding of past climatic and environmental change.

## 1 Introduction

Paleoenvironmental reconstructions, including reconstructions of past climate, provide a powerful tool to document the sensitivity of Earth systems to forcing, characterize the range of natural responses associated with different modes of global change, and identify key mechanisms governing these responses. Throughout the vast majority of the planet’s history, however,

estimates of environmental conditions can only be obtained through proxy reconstructions. The word proxy is derived from the Latin word *procurare*, which in this context means ‘to care’ or ‘to manage’. The measurable physico-chemical quantity in sediments is thus ‘managed’ into a parameter we want to reconstruct. As implied, the result is an indirect estimate of past environmental conditions, often subject to substantial, sometimes poorly characterized, uncertainty.

The simplest proxy reconstructions typically focus on a single environmental variable of interest. Experimental or natural calibration datasets are used to calibrate mathematical relationships between the environmental variable and proxy measure, and these relationships are inverted to obtain quantitative estimates of that variable. Residual variance in the calibration is treated as noise. In reality, however, no proxy exists that is sensitive only to a single paleoenvironmentally-relevant variable, and a large part of the proxy system noise reflects the uncharacterized influence of other environmental and post-depositional variables. Fossil leaf assemblages, for example, exhibit variability that can be associated with mean annual air temperature, but also may be influenced by many other environmental variables and evolutionary history (Royer et al., 2005; Greenwood et al., 2004). The saturation state of alkenones produced by marine phytoplankton is a sensitive recorder of water temperature, but characteristics of alkenones preserved in marine sediments are also strongly affected by physiological factors, seasonality of production, and selective degradation (Conte et al., 1998; Conte et al., 2006). (Conte et al., 1998; Conte et al., 2006). Even recently emerging clumped isotope techniques, which are in theory a direct recorder of the temperature of carbonate mineral formation, can be affected by factors such as growth-rate, carbonate system disequilibrium, and poorly constrained, potentially variable offsets between the environment of carbonate formation and more commonly targeted atmospheric temperature conditions (Passey et al., 2010; Affek et al., 2014; Saenger et al., 2012). (Passey et al., 2010; Affek et al., 2014; Saenger et al., 2012).

Failure to recognize and consider the sensitivity of proxies to multiple environmental factors leads to two important problems in traditional proxy interpretations. First, considering only a single environmental variable in our interpretations maximizes the uncertainty in our reconstructions. Uncertainty could be reduced if the influence of other variables is described and constrained. Second, unacknowledged sensitivity to multiple variables creates potential for biased proxy interpretations if variation in these variables is non-random across the reconstruction.

A productive approach to addressing these issues is the use of proxy system models in the interpretation of proxy data (Evans et al., 2013). These models represent an attempt to mathematically describe the complex of environmental, physical, and biological factors that control how environmental signals are sampled, recorded, and preserved in proxy measurements. Recent reviews and perspectives are available discussing the concepts underlying proxy system models and different ways that they have been applied to proxy interpretation, ranging from substitution for empirical calibrations in inverse estimation of environmental signals to formal integration within climate model data assimilation schemes (Evans et al., 2013; Dee et al., 2016). (Evans et al., 2013; Dee et al., 2016). A growing number of proxy system models and modeling systems are being developed (e.g., Tolwinski-Ward et al., 2011; Stoll et al., 2012; Dee et al., 2015). (e.g., Tolwinski-Ward et al., 2011; Stoll et al., 2012; Dee et al., 2015), and useful models span a range of complexity from empirically-constrained regressions to mechanistic, theory-based formulations. Key to any such model is accurate representation of uncertainty in each model component, which

allows even relatively simple, potentially incomplete models to be used to obtain reconstructions with quantifiable uncertainty bounds.

Reducing the uncertainty of quantitative paleoenvironmental reconstructions, however, further requires adding constraints to proxy interpretations. In situations where two or more proxies share sensitivity to common or complimentary environmental variables, it stands to reason that the information provided by each can be used to refine interpretation of the multi-proxy suite. In practice, a variety of approaches have been used. Commonly, multi-proxy integration has been qualitative and focused on confirmation: trends reconstructed using one proxy system are cross-checked against a second, providing increased confidence in the reconstruction where the patterns match and further investigation where they don't (e.g., Grauel et al., 2013; Keating-Bitonti et al., 2011; Zachos et al., 2006). In other cases, proxies have been combined quantitatively, but usually in a stepwise fashion: one proxy system is used to reconstruct an environmental variable to which it is sensitive, and those reconstructed values are then used to constrain the interpretation of a second proxy (e.g., Fricke et al., 1998; Lear et al., 2000). Although it provides a simple strategy to combining complimentary proxy information, this approach does not fully leverage overlapping information that may be contained in multiple systems that respond to common forcing, is not conducive to robust quantification of uncertainty, and requires that both proxies sample coeval paleoenvironmental conditions.

Here we propose a general approach to proxy interpretation that leverages the benefits of proxy models and provides a robust statistical basis for multi-proxy integration. The method, which we call Joint Proxy Inversion (JPI), couples proxy models with simple environmental time series models representing paleoenvironmental target variables in a Bayesian hierarchical modeling framework (Fig. 1). The hierarchical model is then inverted using Markov Chain Monte Carlo methods (Geman and Geman, 1984) to obtain posterior parameter estimates and paleoenvironmental time series that are conditioned simultaneously on all proxy and calibration data. Similar approaches have been applied in a limited number of cases to conduct large-scale meta-analyses (Tingley and Huybers, 2010; Li et al., 2010; Tingley et al., 2012). We begin by describing an implementation of JPI for the widely-used foraminiferal Mg/Ca and  $\delta^{18}\text{O}$  multi-proxy system, and then present results demonstrating many of the merits and challenges of this approach. The examples are not intended to probe a particularly challenging application or to formally test or validate the approach, but rather to illustrate how JPI offers a robust, accessible framework for the types of quantitative proxy data interpretations routinely conducted within the paleoenvironmental research community.

## 2 Methods

### 2.1 Data

Proxy and proxy model calibration datasets were compiled from published work (Fig. 1). Estimates from fluid inclusions, calcite veins, large foraminifera, and echinoderm fossils (Dickson, 2002; Coggon et al., 2010; Lowenstein et al., 2001; Evans et

~~al., 2018; Horita et al., 2002)~~(Dickson, 2002; Coggon et al., 2010; Lowenstein et al., 2001; Evans et al., 2018; Horita et al., 2002) were combined with information on modern seawater Mg/Ca (de Villiers and Nelson, 1999) to represent variation in seawater Mg/Ca since 80 Ma. For simplicity, and because of the relatively low sensitivity of the other paleoenvironmental variables to seawater Mg/Ca estimates, we use interpreted seawater Mg/Ca estimates given by these authors instead of developing formal models for each Mg/Ca proxy system. Because uncertainty exists in the form of the partitioning function between seawater and echinoderm carbonate, our dataset includes both the original estimates from Dickson (2002) and the reinterpreted estimates of Hasiuk and Lohmann (2010). The uncertainty associated with each estimate was approximated from the primary publication, and ranged from 0.03 mol/mol for modern seawater to ~0.5 mol/mol for some of the proxy estimates (1  $\sigma$ , see data and code available at [https://github.com/SPATIAL-Lab/JPI\\_marine](https://github.com/SPATIAL-Lab/JPI_marine)).

Foraminiferal Mg/Ca and  $\delta^{18}\text{O}$  data were compiled from three Ocean Drilling Program (ODP) sites: site 806, Ontong Java Plateau (~~Lear et al., 2015; Lear et al., 2003; Bickert et al., 1993~~)(Lear et al., 2015; Lear et al., 2003; Bickert et al., 1993); site 1123, Chatham Rise (Elderfield et al., 2012), and site U1385, Iberian Margin (Birner et al., 2016). All Mg/Ca data are all derived from infaunal foraminifera, which exhibit little to no Mg/Ca sensitivity to changing bottom water saturation state (Elderfield et al., 2010). Data from site 806 constitute a low-resolution record from ~18 Ma to present, with an average sampling resolution of 1 sample per 240 and 180 kyr for Mg/Ca and  $\delta^{18}\text{O}$ , respectively, prior to 800 ka (sampling for  $\delta^{18}\text{O}$ , in particular, increases several fold thereafter). Mg/Ca measurements were made on *Oridorsalis umbonatus*, and  $\delta^{18}\text{O}$  data represent the benthic genus *Cibicidoides*. For the other two sites, data were extracted for the overlapping period (1.32 – 1.23 Ma) and comprise a set of higher-resolution records (sampling resolution between 1 per 110 and 1 per 1,700 years across both proxies) spanning two glacial/interglacial cycles. Mg/Ca measurements were made on tests of *Uvigerina* spp at both sites, and  $\delta^{18}\text{O}$  data are from either *Uvigerina* spp (site 1123) or *Cibicidoides wuellerstorfi* (site U1385). Variance in the foraminiferal data, e.g., due to analytical effects and sample heterogeneity, was not estimated independently but rather treated as a model parameter and conditioned on the calibration and proxy data.

Calibration datasets were compiled to constrain the Mg/Ca and  $\delta^{18}\text{O}$  proxy system models. Mg/Ca calibration data for *O. umbonatus* are from the compilation of Lear et al. (2015), and include both modern core-top samples and samples from Paleocene and Eocene sediments of ODP site 690B. Data from site 690B include an adjustment for differences in cleaning procedures used for those samples (Lear et al., 2015). For *Uvigerina* spp our reconstructions are based on core-top calibration samples compiled by Elderfield et al. (2010). We also evaluated the now widely-used down-core calibration proposed by Elderfield et al. (2010), which optimizes the foraminiferal Mg/Ca temperature sensitivity to match Holocene to Last Glacial Maximum temperature change inferred from foraminiferal  $\delta^{18}\text{O}$  values and independent constraints on seawater  $\delta^{18}\text{O}$  change. We found that this approach provided relatively weak constraints on the Mg/Ca proxy model parameters and posterior parameter estimates that were entirely consistent with the stronger constraints obtained from core-top calibration (Fig. S1). Including both calibration datasets in JPI produced results similar to the core-top-only approach; as a result, we exclude the down-core calibration for simplicity, but note that multiple calibration approaches can be integrated and/or evaluated within JPI. Each Mg/Ca datum is accompanied by a bottom water temperature (BWT) estimate based on syntheses of observational

data (modern) or  $\delta^{18}\text{O}$  thermometry (paleo), the latter assuming ice-free conditions. ~~We adopt both sets of estimates directly, applying a normally distributed uncertainty to the BWT values with a standard deviation of 0.2 and 1 °C for the modern and paleo data, respectively, to approximate the different quality of these estimates. (Lear et al., 2015). We adopt both sets of estimates directly. Given that systematic uncertainty estimates for the BWT values are not available, we approximate these~~  
 5 ~~uncertainties as normally distributed with standard deviations of 0.2 and 1 °C for the modern and paleo data, respectively. These values represent rough estimates of the average uncertainty associated with each data type, based on the primary data sources.~~

For  $\delta^{18}\text{O}$  we used the compilation of Marchitto et al. (2014) including new and published coretop data for the genera *Cibicoides* and *Uvigerina* ~~(Keigwin, 1998; Grossman and Ku, 1986; Shackleton, 1974).~~ ~~(Keigwin, 1998; Grossman and Ku,~~  
 10 ~~1986; Shackleton, 1974).~~ Estimates of BWT and  $\delta^{18}\text{O}$  of seawater from the original authors were adopted with an estimated uncertainty of 0.2 °C (1  $\sigma$ ) for BWT; as for Mg/Ca we do not attempt to constrain the uncertainty in the relationship between temperature and  $\delta^{18}\text{O}$  fractionation between seawater and calcite directly, but treat it as a model parameter.

The age of each pre-modern datum was taken from the primary source. Age uncertainties, where known, can be incorporated in the JPI analysis framework by treating ages as random variables rather than as fixed values and/or including  
 15 proxy model components representing processes governing the time-integration of observations. For simplicity, we do not include such a treatment here. In the discussion we note examples where including age uncertainty would produce a more robust analysis.

## 2.2 Proxy models

The proxy system models comprise the ‘data model’ layer of the hierarchical model, representing how environmental signals  
 20 are embedded in the paleo-proxy and proxy calibration data. The models used here are comprised of simple transfer functions relating proxy data to contemporaneous environmental variables, and as such can be considered “sensor models” in the terminology of Evans et al. (2013). ~~, with aspects of proxy signal integration and sampling treated in the “archive” and “observation” models of those authors being swept into the error terms of our data model equations (1-3).~~ The simplest model is that for seawater Mg/Ca proxy data, where, as noted above, we consider the interpreted data directly, giving:

$$MgCa_{swp}(i) \sim N[MgCa_{sw}(t_{swp}[i]), \sigma_{swp}(i)]. \quad \text{Eq. (1)}$$

Here  $MgCa_{swp}(i)$  is the  $i^{\text{th}}$  proxy estimate,  $N$  represents the normal distribution,  $MgCa_{sw}$  is the paleo-seawater Mg/Ca value, and  $t_{swp}$  and  $\sigma_{swp}$  are the estimated age estimate and uncertainty, respectively, associated with a proxy estimate observation.

30 We model foraminiferal Mg/Ca ( $MgCa_f$ , including both calibration and proxy data) as a function of seawater chemistry and bottom water temperature. ~~, using the widely-applied linear form for temperature sensitivity (Elderfield et al., 2010; Bryan and Marchitto, 2008; Lear et al., 2015):~~

$$MgCa_f(i) \sim N\left[\left(\alpha_1 + \alpha_2 \times BWT[t_{MgCaf}(i)]\right) \times MgCa_{sw}(t_{MgCaf}[i])^{\alpha_3}, \tau_{MgCaf}\right] \left[\alpha_1 + \alpha_2 \times BWT(t_{MgCaf}[i])\right] \times MgCa_{sw}(t_{MgCaf}[i])^{\alpha_3}, \tau_{MgCaf}], \quad \text{Eq. (2)}$$

where  $\alpha_{1-3}$  and  $\tau_{MgCaf}$  are the parameters and precision ( $1/\sigma^2$ ) associated with the transfer function, respectively, and other parameters are analogous to equation 1. Experiments conducted using the also-common exponential form produced similar results. In the absence of theoretical constraints, we assign normally distributed priors to the  $\alpha$  parameters based on Bayesian regression of the expression for the mean in equation 2 against the calibration datasets. ~~For *Oridorsalis* we assume paleo-seawater Mg/Ca of 1.5 mol/mol in the Paleocene and Eocene for these initial estimates, and the prior estimates are  $\alpha_1 \sim N[1.5, \sigma = 0.1]$ ,  $\alpha_2 \sim N[0.1, \sigma = 0.01]$ , and  $\alpha_3 \sim N[-0.02, \sigma = 0.03]$ . For *Uvigerina* these distributions are  $\alpha_1 \sim N[1.02, \sigma = 0.1]$  and  $\alpha_2 \sim N[0.07, \sigma = 0.01]$ , and the prior estimated for  $\alpha_3$  from the *Oridorsalis* data set was used.~~ These independent regression estimates, used only to specify the prior probability of the model parameters in the full analysis, require an estimate of Paleocene-Eocene Mg/Ca for the *Oridorsalis* calibration; we use a value of 1.5 mol/mol (Lear et al., 2015). This gives values of  $\alpha_1 \sim N[1.5, \sigma = 0.1]$ ,  $\alpha_2 \sim N[0.1, \sigma = 0.01]$ , and  $\alpha_3 \sim N[-0.02, \sigma = 0.03]$  for *Oridorsalis* and  $\alpha_1 \sim N[1.02, \sigma = 0.1]$  and  $\alpha_2 \sim N[0.07, \sigma = 0.01]$  for *Uvigerina*. We apply the  $\alpha_3$  prior estimated from the *Oridorsalis* data set to *Uvigerina* because no calibration data were available representing non-modern  $MgCa_{sw}$ . For both genera, the prior estimate on the precision of the foraminiferal Mg/Ca model,  $\tau_{MgCaf}$ , is the gamma distribution  $\Gamma[\text{shape} = 2, \text{rate} = 1/30]$ , which approximates the precision of the independent regressions.

Foraminiferal calibration and proxy  $\delta^{18}O$  values ( $\delta^{18}O_f$ ) are modeled similarly, ~~with using the standard 2<sup>nd</sup> order temperature sensitivity equation (Marchitto et al., 2014; Shackleton, 1974) applied in most paleoceanographic work:~~

$$\delta^{18}O_f(i) \sim N\left[\left(\delta^{18}O_{sw}(t_{\delta 180f}[i]) + \beta_1 + \beta_2 BWT[t_{\delta 180f}(i)] + \beta_3 BWT[t_{\delta 180f}(i)]^2, \tau_{\delta 180f}(i)\right) \left[\delta^{18}O_{sw}(t_{\delta 180f}[i]) + \beta_1 + \beta_2 BWT(t_{\delta 180f}[i]) + \beta_3 BWT(t_{\delta 180f}[i])^2, \tau_{\delta 180f}(i)\right]. \quad \text{Eq. (3)}$$

Here  $\delta^{18}O_{sw}$  is the modeled seawater isotope composition and  $\beta_{1-3}$  are the transfer function coefficients. In this analysis we treat the scale conversion factor between the SMOW and PDB reference scales (Shackleton, 1974) as implicit in the transfer function intercept term ( $\beta_1$ ), which is relevant only in comparing our posterior parameter estimates to other work. Prior estimates of the model parameters were obtained and specified as for Mg/Ca; these are  $\beta_1 \sim N[3.32, \sigma = 0.02]$ ,  $\beta_2 \sim N[-0.237, \sigma = 0.01]$ ,  $\beta_3 \sim N[0.001, \sigma = 0.0005]$  for *Cibicidoides* and  $\beta_1 \sim N[4.05, \sigma = 0.06]$ ,  $\beta_2 \sim N[-0.215, \sigma = 0.02]$ ,  $\beta_3 \sim N[-0.001, \sigma = 0.001]$  for *Uvigerina*. Because our analysis focuses on Myr-scale trends and the amplitude of high-frequency (i.e. below the resolution of our model)  $\delta^{18}O_{sw}$  variance in the record from site 806 increased substantially with the onset of modern, 100 kyr glacial cycles, we modeled  $\tau_{\delta 180f}(i)$  separately for proxy data younger than 800 ka (prior on  $\tau_{\delta 180f} \sim \Gamma[6, 1]$ ) and for all other proxy and calibration data ( $\Gamma[3, 1/30]$ ). The former estimate is based on the observed proxy variance since 800 ka, whereas the latter approximates the precision of the calibration relationships. Alternatively, if reconstruction of sub-Myr variability in this part



of the record was a target, the change in properties of the  $\delta^{18}O_{sw}$  record could be represented by addition of a periodic model component in the environmental time series model.

### 2.3 Environmental models

Although not treated as such in most reconstructions, paleoenvironmental conditions are autocorrelated in time, meaning that each proxy observation provides information about conditions not just at a single point in time but across a segment of time. To reflect this, we model paleoenvironmental variables as time series using a correlated random walk model. This parameterization is desirable in that it is minimally prescriptive (i.e. no preferred state or pattern of change is proscribed) but allows incorporation of constraints on (and extraction of inference about) two basic characteristics of the paleoenvironmental system – namely its rate and directedness of change. The environmental models represent the “process model” layer of the Bayesian hierarchical model.

The continuous-time correlated random walk for variable  $Y$  (where  $Y$  is  $MgCa_{sw}$ ,  $\delta^{18}O_{sw}$ , or  $BWT$ ) is expressed as:

$$Y(t) = Y(t - 1) + \epsilon_Y(t), \quad \text{Eq. (4)}$$

where:

$$\epsilon_Y(t) = N[\phi_Y \times \epsilon_Y(t-1), \tau_Y] \left[ \epsilon_Y(t-1) \times \phi_Y^{\Delta t}, \frac{(1-\phi_Y^2)\tau_Y}{(1-\phi_Y^{2\Delta t})} \right]$$

Eq. (5)

In short, the variable follows a random walk in which the next value in the time series is a function only of the current time step size ( $\Delta t$ ), the current value, and a normally distributed error term  $\epsilon_Y$ , which has a temporal autocorrelation of  $\phi_Y$  and precision  $\tau_Y$ . This gives three independent parameters,  $\phi_Y$ ,  $\tau_Y$ , and an initial value of  $Y$  at the beginning of the time series. Each variable is modeled on a time series composed of a regularly-spaced base series appropriate to the record duration and resolution plus all proxy sample ages. We do not explicitly model the covariance among environmental variables, but let this emerge from the data.

For seawater Mg/Ca, which is thought to evolve gradually (the oceanic residence times of Mg and Ca are 13 Ma and 1 Ma, respectively) in response to long-term tectonic and biogeochemical forcing (Wilkinson and Algeo, 1989), we simulate the time use a base series at 1 Myr steps from 80 Ma to present. Although the foraminiferal proxy data used here span only the interval from ~18 Ma to present, extending the seawater model over this longer temporal domain was necessary in order to generate a stable time series, conditioned on sparse seawater Mg/Ca proxy data, that spanned both the proxy records and the Paleogene-aged Mg/Ca proxy calibration data. Given that the modeled quantity is a ratio, we treat the error term in this time series model as a proportion, such that the change in  $MgCa_{sw}$  between two time steps is  $MgCa_{sw}(t-1) * \epsilon_{MgCa_{sw}}$ . We adopt

priors that imply relatively slow change and strong temporal trends ( $\phi_{MgCa_{sw}}$  is given by a uniform distribution,  $U[0.9, 1]$ ;  $\tau_{MgCa_{sw}} \sim \Gamma[100, 0.01]$ ). We use a weak prior on the initial state of  $MgCa_{sw}$  at 80 Ma,  $U[1, 3]$ , consistent with independent interpretations of Cretaceous proxy data (Coggon et al., 2010).

We select the bounds, base resolution, and prior distributions for the bottom water temperature and  $\delta^{18}O$  time series models based on the properties of each record. For site 806 we use a time-step-base series of 50 kyr steps from 18 Ma to present, adequate to allow the time series model to adapt across the range of supra-orbital timescales represented in the sample distribution. Prior estimates of the error term parameters were chosen to allow sampling across a range of weak to moderate all possible autocorrelation states and and a range of error variances that were consistent with first-order interpretations of the proxy data ( $\phi \sim U[0, 0.41]$  for both proxies;  $\tau_{BWT} \sim \Gamma[20, 20.1]$ ;  $\tau_{\delta^{18}O_{sw}} \sim \Gamma[4030, 0.201]$ ). We use weakly informative uniform priors for initial values at 18 Ma ( $BWT(-18) \sim U[3, 8]$ ,  $\delta^{18}O_{sw}(-18) \sim U[-1, 1]$ ). For the higher-resolution Pleistocene records, we bound the models between 1.32 and 1.235 Ma and adopt a time-step-base series of 1 kyr steps, accommodating orbital time-scale changes in the paleoenvironmental variables. We, and adopt the same prior distributions for  $\tau_{BWT}$  and  $\tau_{\delta^{18}O_{sw}}$  as in the long-term model, but use a broader prior on  $\phi$  ( $U[0, 0.8]$  for both environmental variables) based on the expectation that temporal autocorrelation in temperature and seawater  $\delta^{18}O$  trends may be stronger at timescales of 1 kyr than at 50 kyr.

## 2.4 Model inversion

The model structure described above was coded in the BUGS (Bayesian inference Using Gibbs Sampling) language (Lunn et al., 2012) and Markov Chain Monte Carlo was used to generate samples from the posterior distribution of all model parameters conditioned on the proxy and calibration datasets. The analysis was implemented in R version 3.5.1 (R Core Team, 2018) using the rjags (Plummer, 2018) and R2jags (Su and Yajima, 2015) packages. Three chains were run in parallel. Convergence was assessed visually via trace plots and with reference to the Gelman and Rubin convergence factor (Rhat; Gelman and Rubin, 1992) and effective sample sizes reported by rjags.

For the site 806 analysis, nine chains were run to a length of  $1.5 \times 10^6$  samples with a burn-in period of  $10^5$  samples and thinning to retain a total of 5,000,150 posterior samples per chain. All parameters showed strong convergence (Rhat < 1.05, effective sample size > 3,500) with the exception of some parts of the seawater Mg/Ca time series and the initialization period of the BWT and  $\delta^{18}O_{sw}$  time series (i.e. prior to the first proxy observation). The long run and burn-in periods were dictated by the  $MgCa_{sw}$  time series values, which exhibited was characterized by very strong autocorrelation as a result of their ‘stiff’ time series behavior and weak data constraints. Qualitative assessment showed no perceptible covariance between seawater Mg/Ca and other parameters in the posterior samples, nor was the posterior distribution obtained from this inversion substantially different from one produced by inverting the Mg/Ca proxy model alone (which was run to an effective sample size >4,000 beyond the initialization period); as a result, we do not believe the weaker sampling from the  $MgCa_{sw}$  posterior has a significant impact on our results or interpretations. The entire analysis took approximately 2236 hours running on threenine cores of a Windows desktop computer.

For the Pleistocene data we conducted three different analyses, the first two inverting data from each site independently and the third inverting both records together. For the joint inversion of both records, we treated each paleoenvironmental timeseries as independent, i.e. no correlation structure was imposed on or fit to the conditions simulated at the two sites, and the model consists of four time series process models (one each for  $BWT$  and  $\delta^{18}O_{sw}$  at each site) and a single set of data models for the foraminiferal  $Mg/Ca$  and  $\delta^{18}O$  proxy systems. A more comprehensive analysis could include cross-site paleoenvironmental correlation, e.g., as in Tingley and Huybers (2010), but here we opt for a minimal model form and any evidence for correlation emerges from the proxy data directly. Because of the short time interval covered by these analyses we did not model the seawater  $Mg/Ca$  explicitly, but estimated paleo-seawater  $Mg/Ca$  values, where needed, from the posterior distributions of an independent inversion of the seawater  $Mg/Ca$  proxy data. ~~Chains~~ Three chains were run to  $5e^5$  samples for the single-site analyses and ~~7~~ nine chains to  $2.5e^5$  samples for the ~~single and multi-site analyses, respectively,~~ using a burn in period of  $1e^4$  samples and thinning to retain 5,000 posterior samples per chain. All parameters showed strong convergence ( $Rhat \ll 1.05$ ) and effective samples sizes were  $>4,000$  for most parameters and  $>2,000$  for all parameters excluding the initialization period of the time series (i.e. prior to the first observation). Total analysis time ranged from  $<1$  hour (site 1123) to  $\sim 4$  ~~hours running three chains in parallel days (multi-site).~~

Run times for all analyses can be substantially reduced by adopting a smaller number of time steps (e.g., only the base series) and using interpolation to estimate environmental parameter values at the proxy observation time-points. Results from experiments using this approach (not shown) were not detectably different from those shown here.

### 3 Results and Discussion

#### 3.1 JPI paleoenvironmental reconstructions

The paleoenvironmental reconstructions obtained by applying JPI to the site 806 data are similar, to first order, to the reconstructions from Lear et al. (2015; hereafter L15) on which our analysis was modeled (Figs. 2 and 3). Our estimates of seawater  $Mg/Ca$  match those obtained by L15 using polynomial curve-fitting throughout most of the common period of analysis (Fig. 2). Prior to 40 Ma our estimates diverge somewhat, reflecting the ~~incorporating~~ additional data used in our analysis, but this difference does not impact other interpretations given that L15 did not use the curve-fit estimates from this part of the record in their analysis work. Our reconstruction shows strong support for  $\sim 2^\circ C$  of bottom-water warming at site 806 during the mid-Miocene Climatic Optimum (centered here on  $\sim 15.5$  Ma), and although abrupt cooling followed this event, water temperatures warmed again by  $\sim 1^\circ C$  into the late Miocene (Fig. 3). A strong and sustained multi-Myr cooling trend began at the site just prior to 5 Ma and persisted throughout the remainder of the record. Our median temperature estimates are most similar to those obtained by L15 using their “NBB” calibrations, which was based on the same compilation of calibration data used here. 95% credible intervals estimated from JPI average  $2.84^\circ C$  and  $0.86\%$ , which is similar to ~~but slightly larger than~~ the uncertainty bounds provided by L15 based on iterative estimation using different calibration functions.

The width of the JPI CIs varies subtly across the time series, with somewhat narrower intervals during periods of dense sampling, e.g., in the late Pleistocene.

JPI paleoenvironmental time series for the single- and multi-site analysis of the Pleistocene data were nearly identical, with slightly broader credible intervals for both parameters (BWT and  $\delta^{18}\text{O}_{\text{sw}}$ ) and sites in the single-site analyses (Figs. S2 and S3). The multi-site analysis showed coherent and slightly phase-shifted patterns of BWT variation across glacial-interglacial cycles at the two sites, with the amplitude of variation being approximately twice as high and median BWT estimates 2 to 5 °C warmer at U1385 (Fig. 4a). Reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  values show greater glacial-scale variability at site 1123, with abrupt decreases of  $\sim 0.5\text{‰}$  accompanying both glacial terminations (Fig. 4b). In contrast, the seawater  $\delta^{18}\text{O}$  time series reconstructed for site U1385 shows little response to the termination at  $\sim 1.295$  Ma and exhibits high-frequency variability not seen at 1123. Both reconstructions are similar in nature to those provided by the original authors. Absolute temperatures and  $\delta^{18}\text{O}_{\text{sw}}$  values match well if the published reconstructions are adjusted using the Mg/Ca proxy sensitivity inferred here (0.068 mmol/mol per degree; Fig. 4); the Elderfield et al. (2010) calibration used by the original authors offsets the warmer site U1385 temperatures from JPI results by as much as ca. -2 °C (Figs. S2 and S3). Neither of these studies presents quantitative uncertainty bounds on individual paleotemperature or  $\delta^{18}\text{O}_{\text{sw}}$  estimates, but both provide estimates of average uncertainty based on propagation of errors. The average width of our 95% CIs is actually somewhat narrower than the  $2\sigma$  values from the original papers, and the JPI CIs are notably narrower for the U1385 record (2.37 °C, 0.6‰) than for 1123 (2.93.3 °C, 0.78‰; all estimates from the multi-site analysis).

### 3.2 Time series properties

One visually striking difference between the JPI and L15 reconstructions is the higher BWT and  $\delta^{18}\text{O}_{\text{sw}}$  variability implied by L15 (Fig. 3). As is common in traditional proxy interpretations, the L15 paleoenvironmental record treats each individual proxy observation as an estimate of an independent environmental state, giving a reconstruction centered on ‘best estimates’ derived from each data point. In reality, however, the environmental states giving rise to the proxy data are not independent if autocorrelation exists at the resolution at which the time series is sampled. For BWT and  $\delta^{18}\text{O}_{\text{sw}}$  this is true over a broad spectrum of temporal resolutions including those considered here; e.g., values of these parameters are known to vary systematically over millions of years due to long-term fluctuations in Neogene climate and ice volume (Zachos et al., 2001; Raymo and Ruddiman, 1992) and over tens to hundreds of thousands of years due to orbital forcing (Imbrie et al., 1984; Shackleton, 2000). This is often implicitly acknowledged in the presentation of traditional proxy reconstructions by including a smoothed representation of the record, obtained using a (usually somewhat arbitrary) filter (e.g., Elderfield et al., 2012).

JPI, in contrast, explicitly considers temporal autocorrelation of the underlying environmental variables, treating each proxy observation as a sample arising from one or more underlying, autocorrelated environmental time series. The properties of the time series themselves, rather than being assumed, are estimated using the proxy models and the data, meaning that the record produced is optimized to reflect the actual smoothed reconstruction reflects the information content of the data. For very

certain proxy models or densely distributed data that record high-frequency variability, the reconstructed time series will express short-term changes in the environment, ~~whereas. In contrast,~~ reconstructions based on uncertain models or ~~smooth or~~ sparsely-sampled data will tend toward greater smoothing and reflect ~~the actual information content of the proxies with respect to~~ the longer-term evolution of the mean state of the system. This is nicely illustrated by comparison of JPI  $\delta^{18}O_{sw}$  reconstructions for sites 1123 and U1385: the sample density of the U1385 proxy record is approximately 15 times greater, and the resultant time series reconstruction expresses much stronger variability at millennial timescales (Fig. 4b). Again, similar results can be achieved using other post-hoc smoothing approaches, but the integration of smoothing, informed by the proxy system model and data properties, within the core data analysis framework is an advantage of JPI.

Another advantage of embedding time series models in JPI is that it offers an explicit framework for integration of differently-sampled proxy records. In most of the studies reviewed here foraminiferal  $\delta^{18}O$  values are more densely sampled than Mg/Ca. In a traditional, piece-wise interpretation of these proxy data,  $\delta^{18}O_{sw}$  can only be estimated if paired oxygen and Mg/Ca data are available for a given core level. Thus, if Mg/Ca data are missing at a level either this value must be estimated, usually through linear interpolation, or the foraminiferal  $\delta^{18}O$  data excluded from the analysis. JPI eliminates the need to exclude or selectively interpolate data by linking all proxy measurements to a common set of continuous time series. The temporal interpolation required to integrate data sampled at different times is conducted for each environmental variable (which are in reality the quantities that are related in time), rather than for the proxy values themselves, as an explicit component of the analysis. One note of caution is warranted here: potential for artefacts to emerge from the integration of datasets with very different sampling densities remains. For example, the high-frequency variability in estimated seawater  $\delta^{18}O$  at site U1385 (Fig. 4b) stems from high-frequency variance in the densely-sampled  $\delta^{18}O_f$  record at this site, but without  $MgCa_f$  at similar resolution it is impossible to determine whether the isotopic proxy record variance truly reflects millennial-scale changes in seawater  $\delta^{18}O$  or instead is driven by un-documented, high-frequency BWT variation.

A final outgrowth of the integration of proxy system and paleoenvironmental time series models via JPI is that the method provides quantitative uncertainty bounds that are linked to and reflect the stratigraphic distribution and density of proxy information. Because environmental parameters are modeled as continuous time series, estimates of central tendency and dispersion (e.g., credible intervals) are obtained throughout the reconstruction period. For time steps in which no observational data are available, the dispersion of posterior estimates increases consistent with the properties of the time series model (e.g., between ~55 and 75 Ma or 5 and 15 Ma in the seawater Mg/Ca model; Fig. 2), providing quantitative estimates of the constraints provided by the data within these intervals. Moreover, because ~~temporal autocorrelation of the environmental variables is considered, densely sampled data, even where samples~~ paleoenvironmental time series are ~~taken~~ temporally autocorrelated, each proxy observation helps constrain the environmental state not just at ~~different~~ the time associated with its stratigraphic levels, ~~place additive constraints on the reconstructed value~~ depth, but also provides (weaker) information about conditions earlier and later in the record (with the decay of that information with time being a function of the ~~environmental state-process model parameters~~). As a result, credible intervals in the posterior distribution adjust ~~to reflect both~~ with the density and the strength of the proxy constraints. The result observations, and stratigraphic intervals with higher sampling density have

lower CIs reflecting the cumulative constraints provided by multiple observations. This can be seen, for example, in the broader 95% CIs for the sparsely-sampled portion of the site 806 record between ~7 and 10 Ma (Fig. 3) or in the contrasting width of the CIs for the two Pleistocene sites (Fig. 4).

### 3.3 Model properties

Bayesian inversion has previously been used to estimate proxy model parameter values in situations where these are poorly constrained (Tolwinski-Ward et al., 2013), and the joint inversion of proxy and environmental time series models performed in JPI can similarly be used to provide constraints on parameter values for all model components- (e.g., Fig. S4). Because the proxy system models used here are simple-~~statistical formulations~~, and the calibration data themselves are used to generate prior estimates on model parameters, the-~~mean~~ posterior estimates are generally quite similar to the priors (Fig. 5). The only notable exception is  $\beta_3$  the second-order parameter in the  $\delta^{18}O_f$  model, for which the posterior mean is shifted subtly toward zero (Fig. 5g). Our prior estimates of parameter variance were slightly inflated to ensure that we did not over-constrain these values, and the posteriors show sharpening of the distributions for most parameters. Posterior estimates for proxy model precision (or variance), however, are much more strongly constrained than those obtained from independent estimation using calibration data only (Figs. 5d and h). We note that our results suggest limited sensitivity of the proxies to some model parameters (e.g.,  $\alpha_3$  and  $\beta_3$ ; Figs. 5c and g). Although this suggests that more parsimonious models omitting these parameters could be used, we retain the ‘canonical’ forms to support comparison with previous work.

These refinements reflect a combination of the constraints offered by the calibration and down-core proxy data. Although at first consideration the relevance of the latter to calibrating proxy model parameters might not be apparent, in fact the proxy model must not only be consistent with the calibration data but also explain the observed proxy data given the ‘true’ environmental conditions. As a result, for a given set of proxy data and environmental time series model properties only a subset of proxy model parameter values will be plausible. Consider, for example, the proxy model precision parameter. In our model construction, this value explains the “noise” both within the model calibration dataset and the proxy record, each of which can arise from a similar ensemble of factors (e.g., temporal variation in the environment at time scales below the time series model time step, biological or random variation in the environment-proxy relationship). Our analysis suggests that before the mid-Pleistocene transition, the proxy model variance implied by the full JPI inversion is similar to that estimated from the calibration data alone (solid curves in Figs. 5d and h), with slightly higher  $\delta^{18}O$  and lower Mg/Ca variance implied by the full analysis. The site 806  $\delta^{18}O_f$  record, however, is much more densely sampled after 800 ka, and the combination of higher  $\delta^{18}O_{sw}$  variability and dense sampling that more strongly records this variability requires a much higher proxy model variance (dashed lines in Fig. 5h). The proxy calibration data offer no constraints on this value, rather the JPI posterior estimates the parameter value to reconcile the environmental time series (representing the longer-term evolution of the mean system state) with the variance expressed in the proxy observations.

Because the JPI analysis involves sampling of all model parameters simultaneously, it also can identify and account for correlation among parameters. The proxy model parameter estimates for site 806 provide a clear example (Fig. 6). The

posterior distributions show strong correlation between the seawater Mg/Ca sensitivity term ( $\alpha_3$ ) and both the intercept and sensitivity terms ( $\alpha_1$  and  $\alpha_2$ ) in the  $MgCa_f$  model and between the first- and second-order terms ( $\beta_2$  and  $\beta_3$ ) in the  $\delta^{18}O_f$  model. This is not at all surprising: in all cases these terms are interactive and for a given estimate of the model calibration a change in one will generally be offset by a change in the other. Accounting for this covariance is important in assessing the uncertainty of proxy reconstructions, however, and may in part account for the more optimistic uncertainty estimates obtained here relative to those based on propagation of errors assuming independence of parameters, in that the latter approach will ~~'double-count'~~inflate uncertainty associated with correlated parameters.

JPI also provides posterior estimates on the environmental time series model parameters, and these distributions can provide information complimentary to the reconstructed time series themselves. Comparing prior and posterior estimates at all three study sites (Fig. 7), the analysis provides strong posterior constraints on the error autocorrelation (i.e. directedness of change)~~)-and-)~~. Posterior estimates of the error variance (i.e. magnitude of change between time steps) for  $\delta^{18}O_{sw}$  and BWT are more similar to the priors, but additional experiments using alternative priors (not shown) suggest that this reflects the appropriateness of the prior estimates and rather than a lack of constraints from the data (i.e. posterior estimates of BWT error variance are only subtly~~distributions were substantially~~ different from the alternative priors~~-(middle column)~~). Interestingly, the error variance estimates are quite similar for both environmental variables at all sites despite the  $\sim 2$  order of magnitude difference in the resolution and length of the ~~time series models and data density records~~, suggesting scale-independence of short-term rates of change in these systems.

In contrast, the error autocorrelation term, which reflects the directedness of environmental change across multiple model time steps, shows substantial variation among the data sets (Fig. 7, left column). The ~~lowest~~highest posterior values (median value  $\sim 0.9$ ) were obtained for the long record at site 806, ~~consistent with the assumption that inertia would be weaker for these variables at the longer time scales (i.e. 50 kyr time steps) reflected in this analysis. Across all scales, posterior distributions for autocorrelation were skewed lower for  $\delta^{18}O_{sw}$  than for BWT. Although this may in part reflect the greater expression of short~~which expresses long-term variance in more densely sampled  $\delta^{18}O_f$  records, the result holds at site 1123, where the sample distributions for  $MgCa_f$  and  $\delta^{18}O_f$  are identical, implying that changes in  $\delta^{18}O_{sw}$  are generally more chaotic than those of BWT. The (multi-Myr), high-amplitude transitions in paleoenvironmental states. Among the Pleistocene analyses, the strongest error autocorrelation is inferred for BWT at site U1385, ~~where~~. There, the data strongly support highly coherent, high-amplitude cyclic variation in BWT across the two glacial cycles sampled. In contrast,  $\delta^{18}O_{sw}$  variation estimated at this site is only weakly directional and features strong, chaotic, millennial-scale variability, reflected in a much lower posterior estimate for error autocorrelation (Fig. 7d).

### 3.4 Derivative analyses

In this final section, we explore additional examples of how JPI results might be used to support inference or hypothesis testing in paleoenvironmental reconstruction. ~~JPI provides a sound basis for testing hypotheses of change within or between proxy records. As with the evaluation of reconstruction uncertainty, the important concept here is that parameter values within~~



individual posterior samples are not independent, but instead reflect the covariance of parameters as constrained by the data and models used. Consider the case where we want to assess the magnitude of change in site 806 bottom water temperature relative to the modern (core top) value. Traditionally, we might take a central estimate of the modern value, e.g., the median shown by the left terminus of the red line in Fig. 8a, and compare it with the reconstructed distribution of values at one or more points in the past to ask whether it is or is not consistent with that distribution. This implicitly assumes that the true environmental parameter values (for modern and the past) are independent of each other, and gives the set of probabilities shown in dotted blue in Fig. 8a. In reality, however, the modern and paleo *BWT* values are not independent, as discussed above. The multivariate posterior samples produced by JPI provide a sound basis for testing hypotheses of change within or between proxy records. Consider the case where we want to assess the magnitude of change in site 806 bottom water temperature relative to the modern (core top) value. Unlike the raw proxy data or traditional interpretations thereof the JPI samples providing distributions for the environmental variables supporting testing at any point in time represented in the paleo-environmental time series. Other interpolation or smoothing methods can and have been used to conduct such tests, for example of change in global temperature relative to modern (Marcott et al., 2013), but an advantage of JPI, again, is that the analysis includes correlation among model parameters and temporal autocorrelation are included and optimized in the analysis, eliminating the need for *ad hoc* methodological choices.

The effect of parameter correlation can account for this by framing the analysis seen in terms of comparing change relative to modern within individual posterior samples (within-sample) versus change between each posterior sample and the 0 Ma median value (between-sample; Fig. 8a, solid blue line). The resulting estimates show interesting, if subtle, contrasts with the latter being equivalent to a traditional approach test for non-zero difference that assumes independence. At short time lags (less than ~400 kyr) the within-sample comparison actually implies somewhat slightly higher probability of significant change. This reflects the influence of error autocorrelation in the time series model: within an individual posterior sample, directional change is likely to persist over multiple time steps, meaning that the ‘signal to noise ratio’ over short periods is higher if estimated based on within-sample vs. between-sample change. Beyond this time frame, however, the relationship between methods inverts, and the traditional method assuming independence gives exaggerated estimates of the significance of change. Beyond the scale of significant time series error autocorrelation, the variance of change estimated from the within-sample comparison is actually slightly substantially greater than that estimated between samples, reflecting the fact that some possible BWT trajectories within the posterior ‘wander’ across the distribution of possible values over time, increasing the dispersion of the change estimates. The net result is that in this case, using a one-sided 95% credible interval threshold (equivalent to  $p=0.05$ ), one would estimate that site 806 bottom water temperatures diverged from modern some 100–200 kyr earlier using the traditional approach than with the more appropriate within sample analysis. 1 Ma earlier without accounting for parameter and time-series correlation.

Another example involves cross-site comparison. Here, we similarly ask whether seawater  $\delta^{18}\text{O}$  values were different at sites 1123 and U1385 throughout the period of study based on comparisons of the posteriors from the multi-site analysis or the two single-site JPI analyses (Fig. 8b). The assessment that assumes independence of estimates at the two sites (the latter



one) consistently under-estimates the significance of the difference between the sites. This can be explained intuitively in terms of the impact of other model parameters on posterior estimates of  $\delta^{18}O_{sw}$  values at both sites. In a given sample from the posterior of the multi-site analysis, if one of the  $\delta^{18}O_f$  proxy system model parameters deviates from the central estimate, for example, it will similarly impact the seawater isotope reconstructions at both sites. As a result, the variance of the between-site differences is reduced in the comparison based on the multi-site analysis, producing stronger results in the post-hoc tests of difference. In this example the choice of approach would have little impact on inferences drawn based on the 95% credible interval, but at the 99% level several parts of the time series would be considered different using the multi-site comparison and not different with the traditional approach (Fig. 8b). Including factors contributing to age model uncertainty for individual records would further improve JPI-based interpretations of this type.

Finally, because JPI results provide integrated, self-consistent estimates of multiple environmental variables, it can be used to identify and characterize multivariate modes of environmental change in Earth's past. Results from the site 806 analysis, for example, demonstrate non-linear coupling between changes in *BWT* and  $\delta^{18}O_{sw}$  since the mid-Miocene (Fig. 9). These patterns, including limited coupling between  $\delta^{18}O_{sw}$  and *BWT* change prior to ~5 Ma and strong bottom water cooling accompanied by a modest  $\delta^{18}O_{sw}$  decrease into the Pleistocene, were previously noted by L15. What is apparent here, however, is the suggestion that the system transitioned between at least three semi-stable states during this time. Jumps between a mid-Miocene warm, low- $\delta^{18}O_{sw}$  state, late Miocene warm, high- $\delta^{18}O_{sw}$  state, and Plio-Pleistocene cool state were in each case relatively abrupt, with the system spending the majority of the reconstruction period within, rather than between, states. ~~Patterns of short term correlation between *BWT* and  $\delta^{18}O_{sw}$  appear to vary among these states, as well, with positive correlation between these variables dominating the first two states and the classical negative correlation characteristic of coupled temperature and ice volume changes only expressed during the final one (Fig. 9, dots).~~

## 4 Conclusion

Traditional approaches to proxy interpretation suffer from broad and poorly characterized uncertainty and potential biases related to the sensitivity of proxies to multiple environmental factors (Sweeney et al., 2018). Proxy system modeling and multi-proxy reconstruction provide partial solutions to these issues, but a robust, accessible framework for integrating these two approaches in the development of paleoenvironmental reconstructions is also needed. We suggest that Bayesian hierarchical models that leverage simple time series representations of paleoenvironmental conditions offer such a framework. This approach is broadly generalizable to any set of proxies for which appropriate forward models can be written. It confers many of the advantages of more complex data assimilation methods that leverage Earth system models (Evans et al., 2013), while remaining independent of the assumptions embedded in these models and flexible enough to be applied over a wide range of systems and time scales. As with any statistically-based analysis, JPI results are model-dependent: they provide a basis for interpreting data in the context of a specific model and its assumptions, and this dependence should be acknowledged and considered in the presentation and interpretation of results.

Our illustration of the method based on the coupled Mg/Ca and  $\delta^{18}\text{O}$  systems in benthic foraminifera demonstrates the flexibility of JPI through applications to two contrasting time scales and both single- and multi-site proxy records. Despite the simplicity of this system and the proxy models used, the example illustrates how JPI can be applied to widely used proxy systems to give improved characterization of uncertainty, explicit estimates of the properties of paleoenvironmental systems, and refined proxy model calibrations. Implementations similar to those demonstrated here could easily and immediately become standard practice in the interpretation of many paleoenvironmental proxy data. As the underlying proxy system models mature, JPI-based interpretations can be revised and refined to incorporate new understanding and/or leverage additional proxy types, minimizing, but also accurately representing, bias and uncertainty in our paleoenvironmental reconstructions.

### **Data and code availability**

- 10 ~~All data and code used to conduct the analyses and create figures reported in this manuscript are available at [https://github.com/SPATIAL-Lab/JPI\\_marine](https://github.com/SPATIAL-Lab/JPI_marine).~~  
All data and code used to conduct the analyses and create figures reported in this manuscript are archived online (Bowen, 2019) and available at <https://doi.org/10.5281/zenodo.3358256>.

### **Author contribution**

- 15 GJB conceived of, designed, and conducted the analyses, with support from BFF, AS, and G-JR. CHL provided access to data and advice on application of the Mg/Ca paleo-thermometer. GJB wrote the manuscript with input from all coauthors.

### **Competing interests**

The authors declare that they have no conflict of interest.

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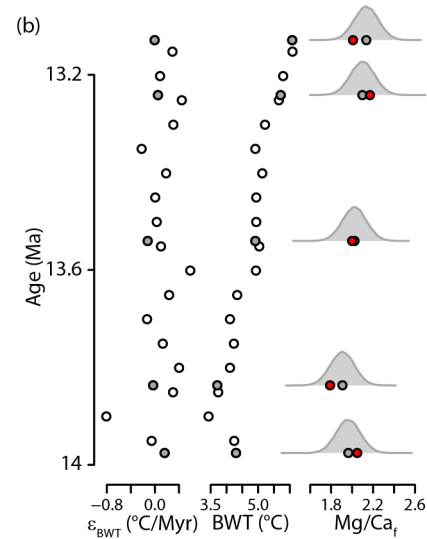
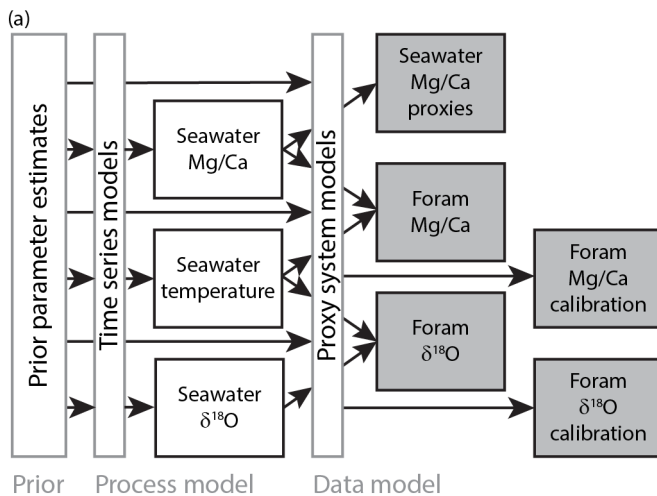
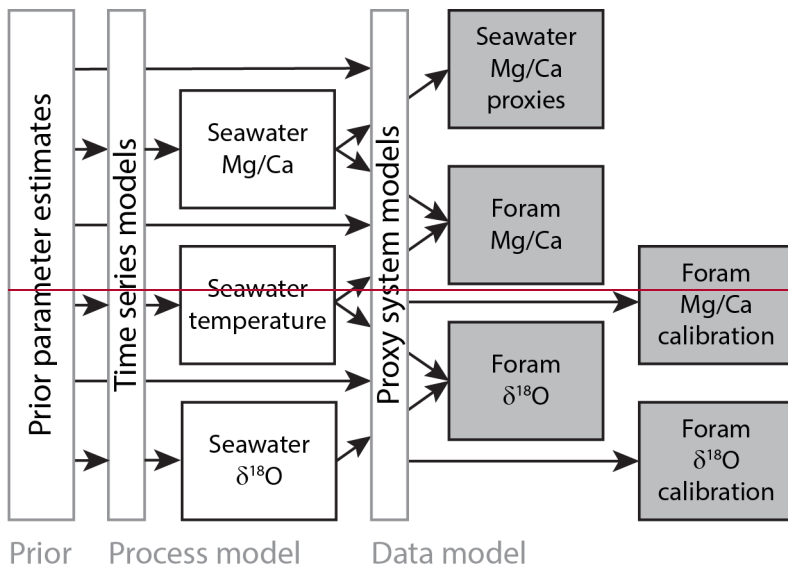
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**Figure 1: Schematic representation of the implementation of JPI for the coupled Mg/Ca and  $\delta^{18}\text{O}$  proxy systems. (a) Schematic. Grey-outlined boxes and text represent the three components of the Bayesian hierarchical model. Markov Chain Monte Carlo sampling is used to ‘explore’ the prior parameter space and develop a statistically representative posterior sample of the parameters and paleoenvironmental time series that are consistent with all paleo proxy and proxy calibration data (grey-filled boxes). (b) Example showing a subset from a single member of the site 690 posterior distribution. Error term values ( $\epsilon_{BWT}$ ) dictate the simulated paleoenvironmental time series trend (in this case  $BWT$ ) modeled at a base frequency (white fill) and all proxy sample levels (grey fill). The environmental state and proxy model parameter values from the posterior sample are used to model the predicted proxy signal (here  $Mg/Ca_i$ , means as grey filled circles and probability density functions as curves). The likelihood of the posterior sample is evaluated based on the probability of the observed proxy data (here foraminiferal  $Mg/Ca$ , red circles) given the modeled values.**

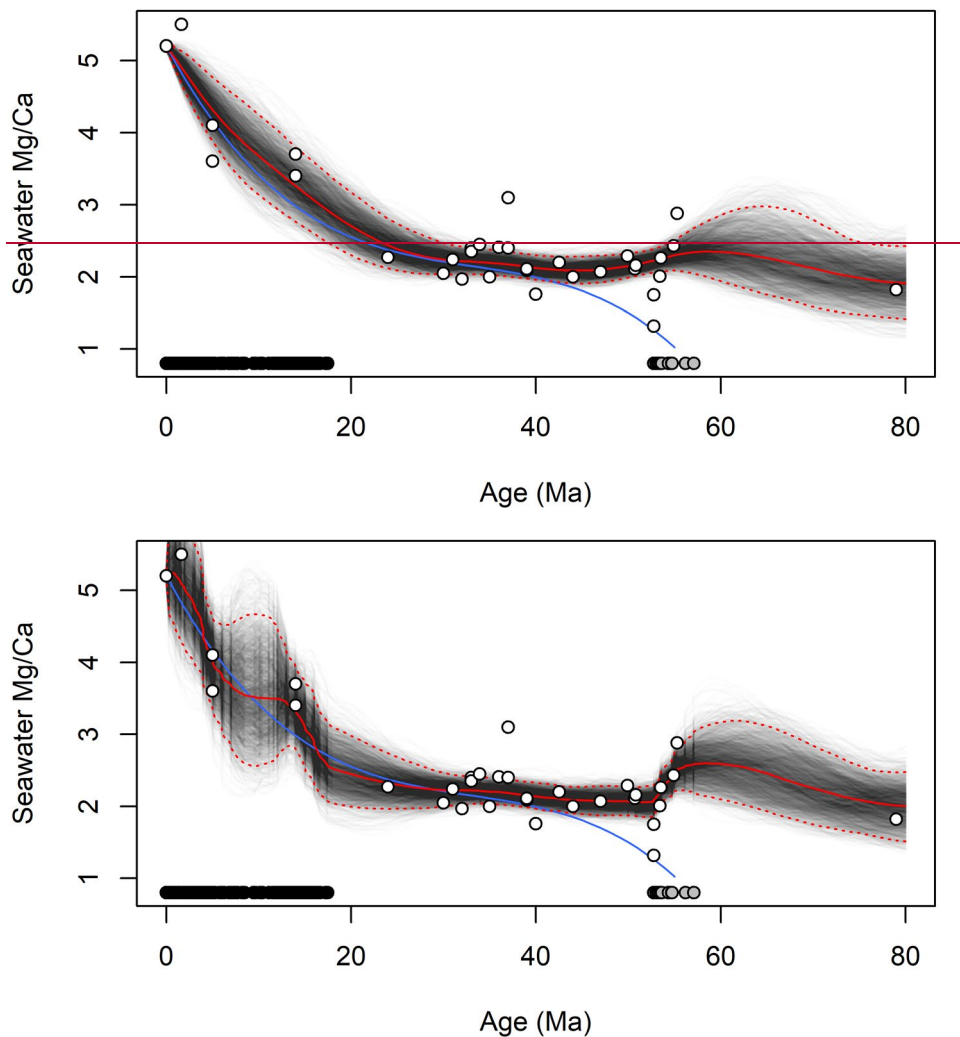
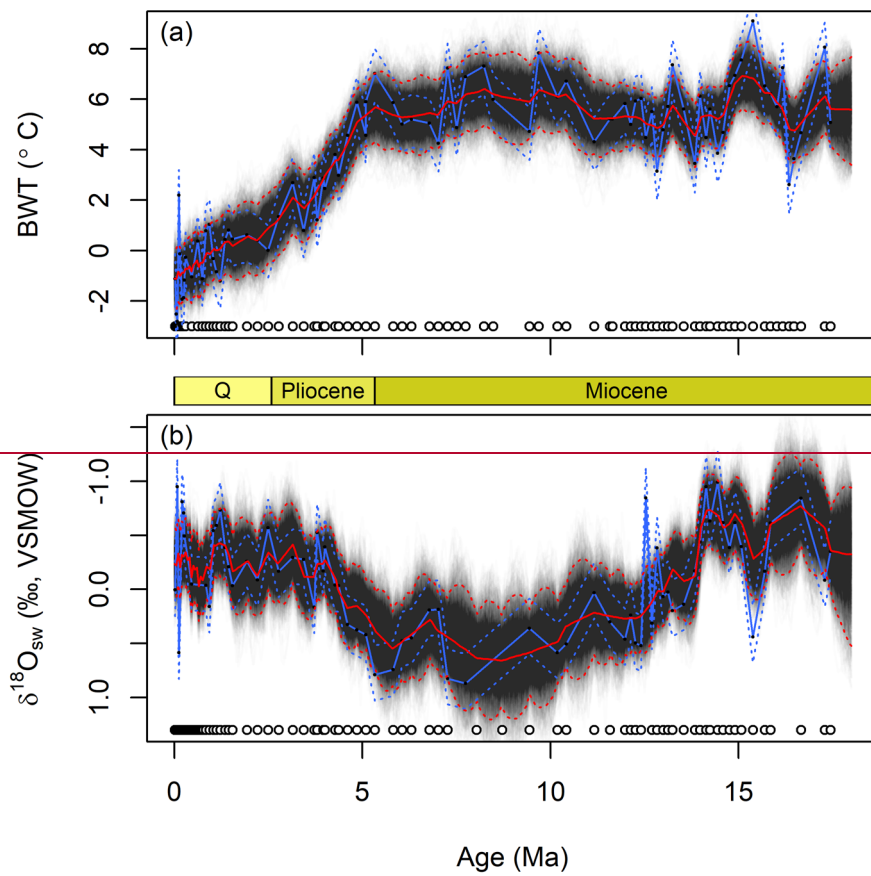


Figure 2: Reconstructed seawater Mg/Ca from 80 Ma to present. Black lines show individual draws from the posterior distribution for each time series; red lines show the median (solid) and 95% credible intervals (dotted). White-filled circles show individual proxy estimates (Dickson, 2002; Coggon et al., 2010; Lowenstein et al., 2001; Evans et al., 2018; Horita et al., 2002; de Villiers and Nelson, 1999), black and grey symbols at the bottom of the panel show the distribution of the foraminiferal Mg/Ca proxy data and Paleogene proxy calibration data, respectively, in time. The blue line is the curve-fit estimate of seawater Mg/Ca of Lear et al. (2015).





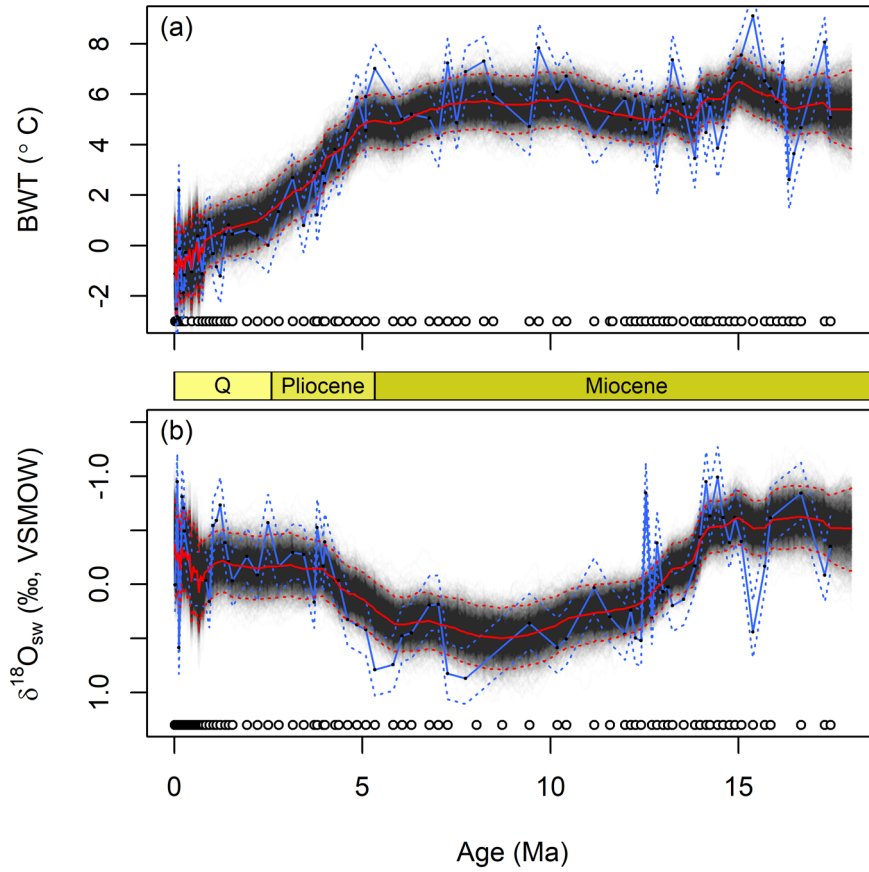
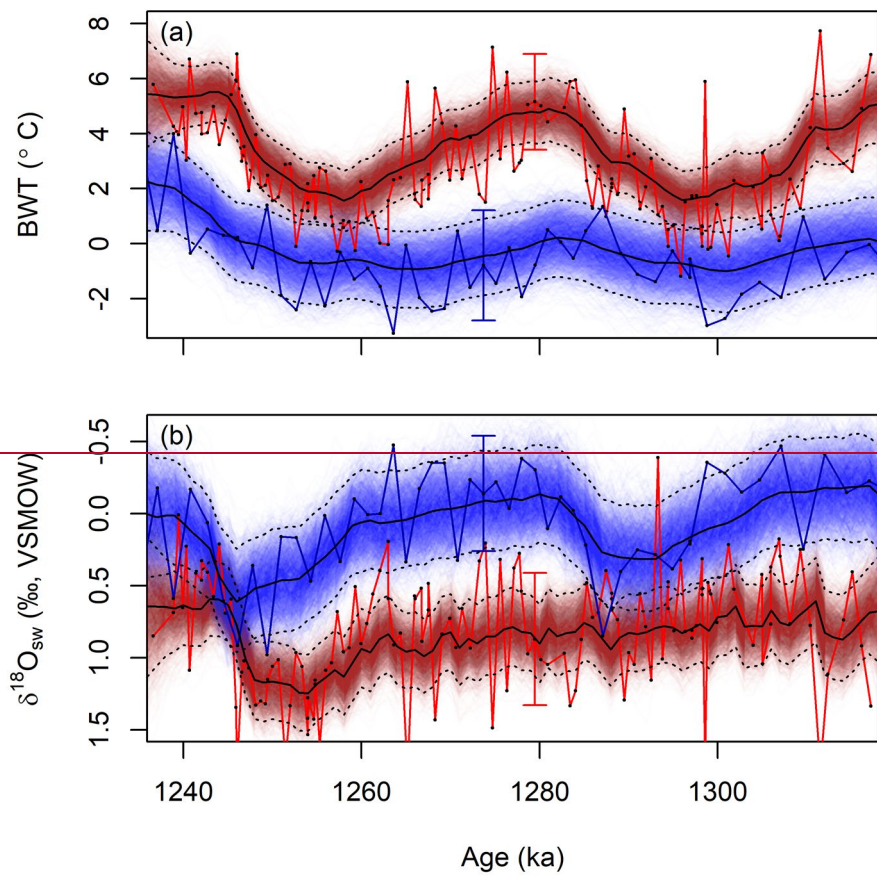
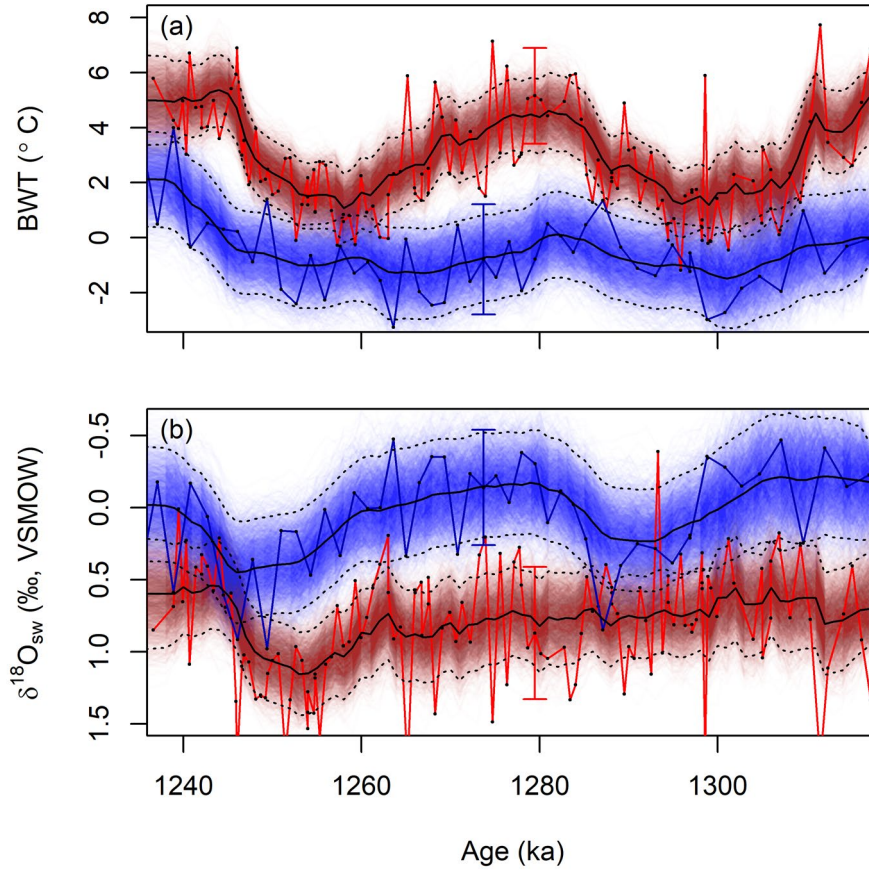
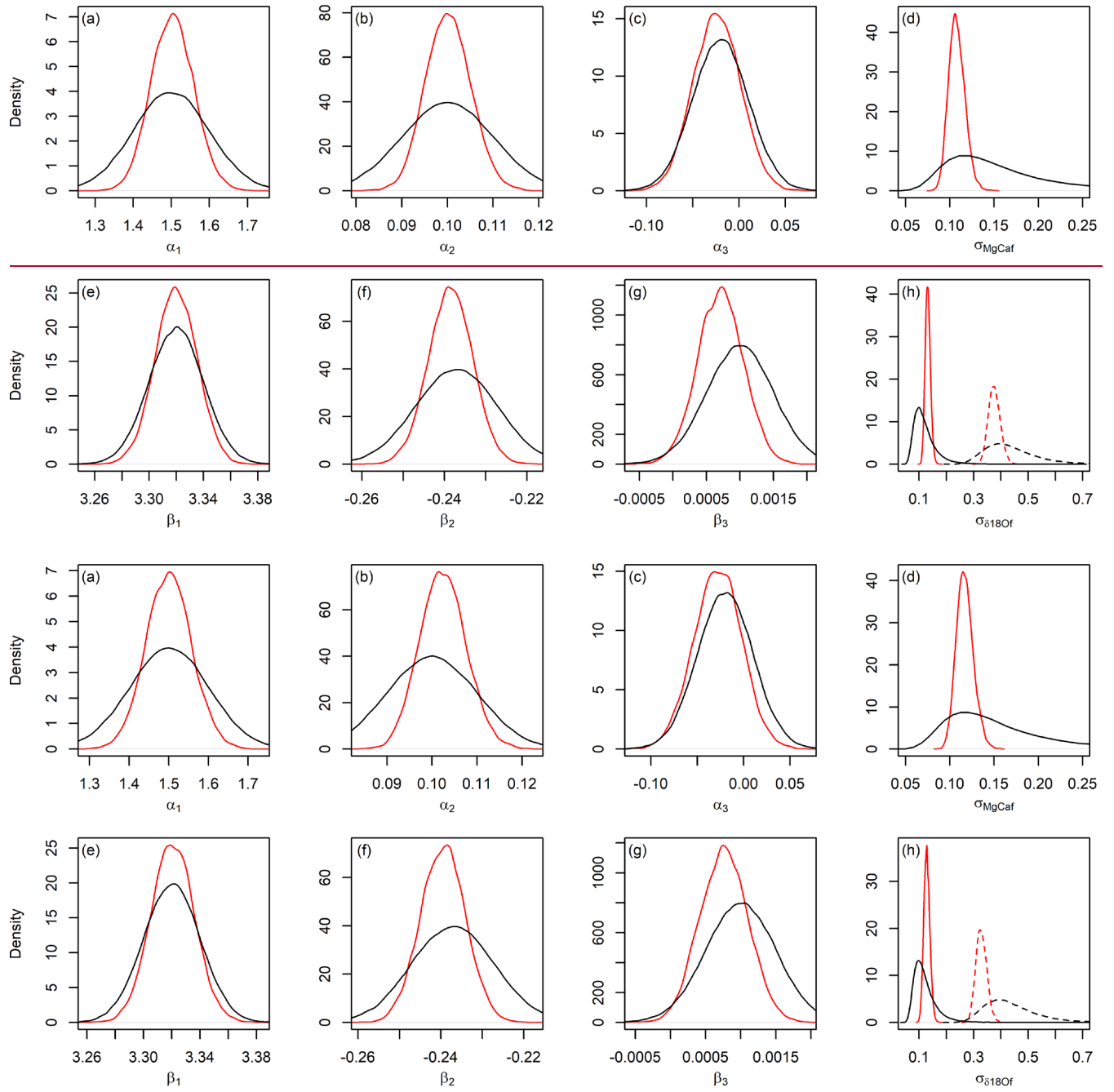


Figure 3: Reconstructed bottom water temperature (a) and seawater  $\delta^{18}\text{O}$  values since 18 Ma (b). Lines as in Fig. 2. Circles show the distribution of foram Mg/Ca (a) and  $\delta^{18}\text{O}$  (b) data in time. Blue lines are the best estimate (solid) and uncertainty envelope (dashed) of the original Lear et al. (2015) interpretation of these data, using their linear “NS-LBB” calibration data set. Q = Quaternary.





**Figure 4: Reconstructed bottom water temperature (a) and  $\delta^{18}\text{O}$  values (b) for sites 1123 (blue) and U1385 (red) based on simultaneous JPI of proxy data from both sites. Symbols as in Fig. 2. Solid red and blue lines show the interpretation of these records as by the original authors (Birner et al., 2016; Elderfield et al., 2012) recalculated using the foraminiferal Mg/Ca temperature sensitivity inferred here. Uncertainty estimates from the original authors ( $2\sigma$ ) are shown as error bars.**



**Figure 5: Prior (black) and posterior (red) distributions for *Oridorsalis umbonatus* Mg/Ca (a-d) and *Cibicides sp.*  $\delta^{18}\text{O}$  (e-h) proxy model parameters (ref. equations 2 and 3, respectively) in the site 806 analysis. Solid and dashed lines in panel H show standard deviations of the calibration relationship prior to and following the 800 ka transition, respectively.**

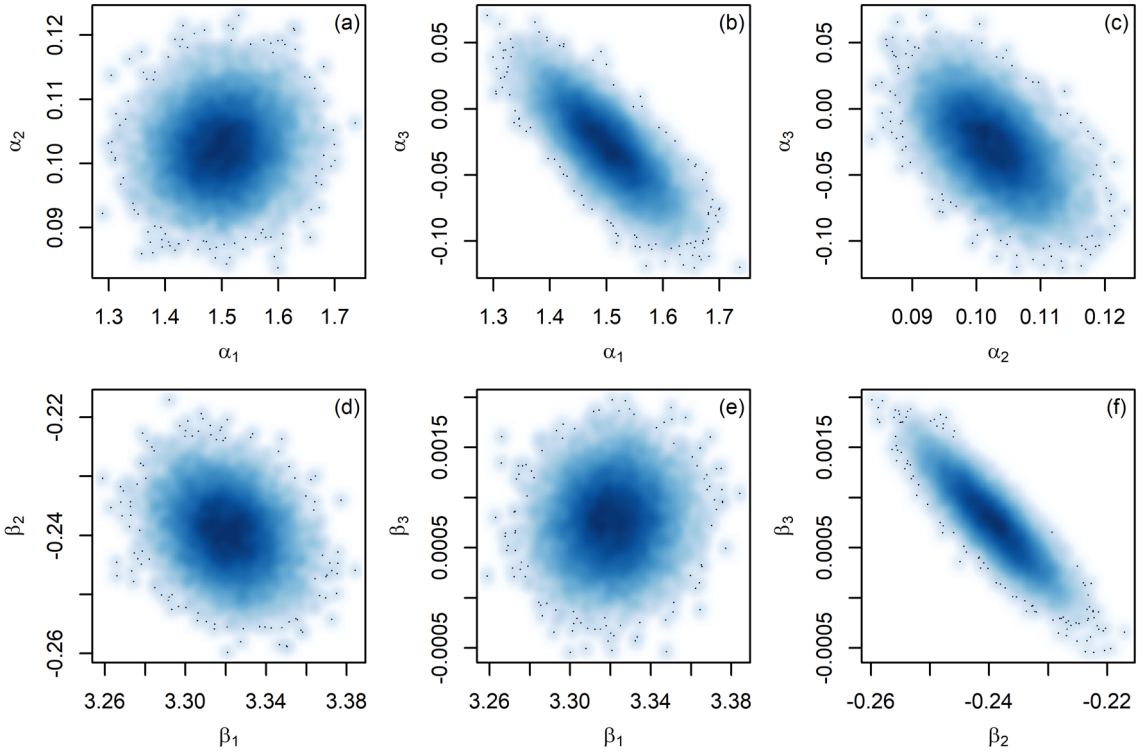
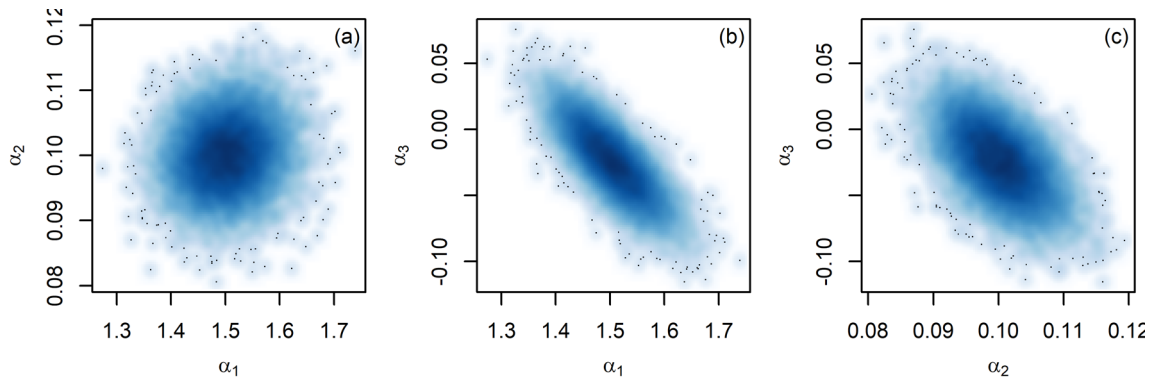
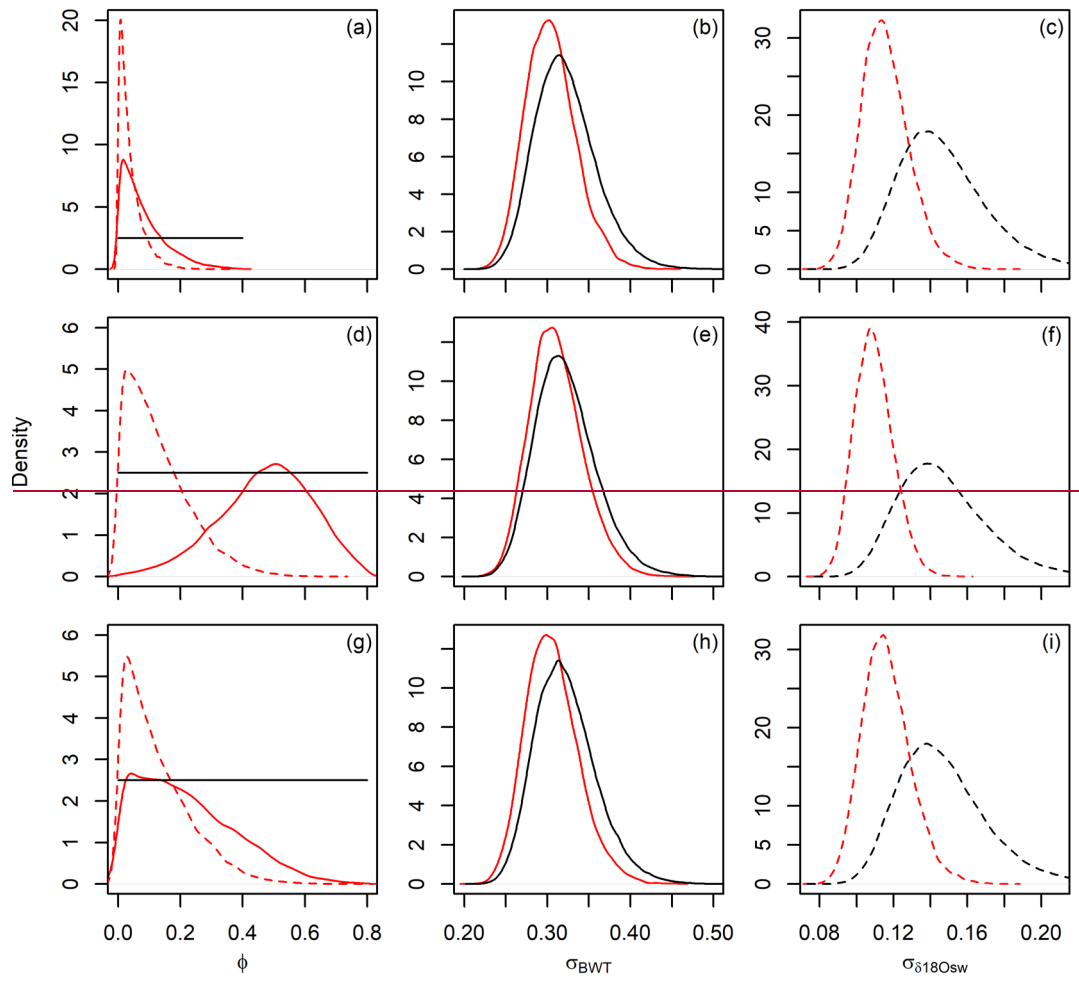


Figure 6: Bivariate density plots of the posterior distributions for *Oridorsalis umbonatus* Mg/Ca (a-c) and *Cibicidoides sp.*  $\delta^{18}\text{O}$  (d-f) proxy model parameters from the site 806 analysis.





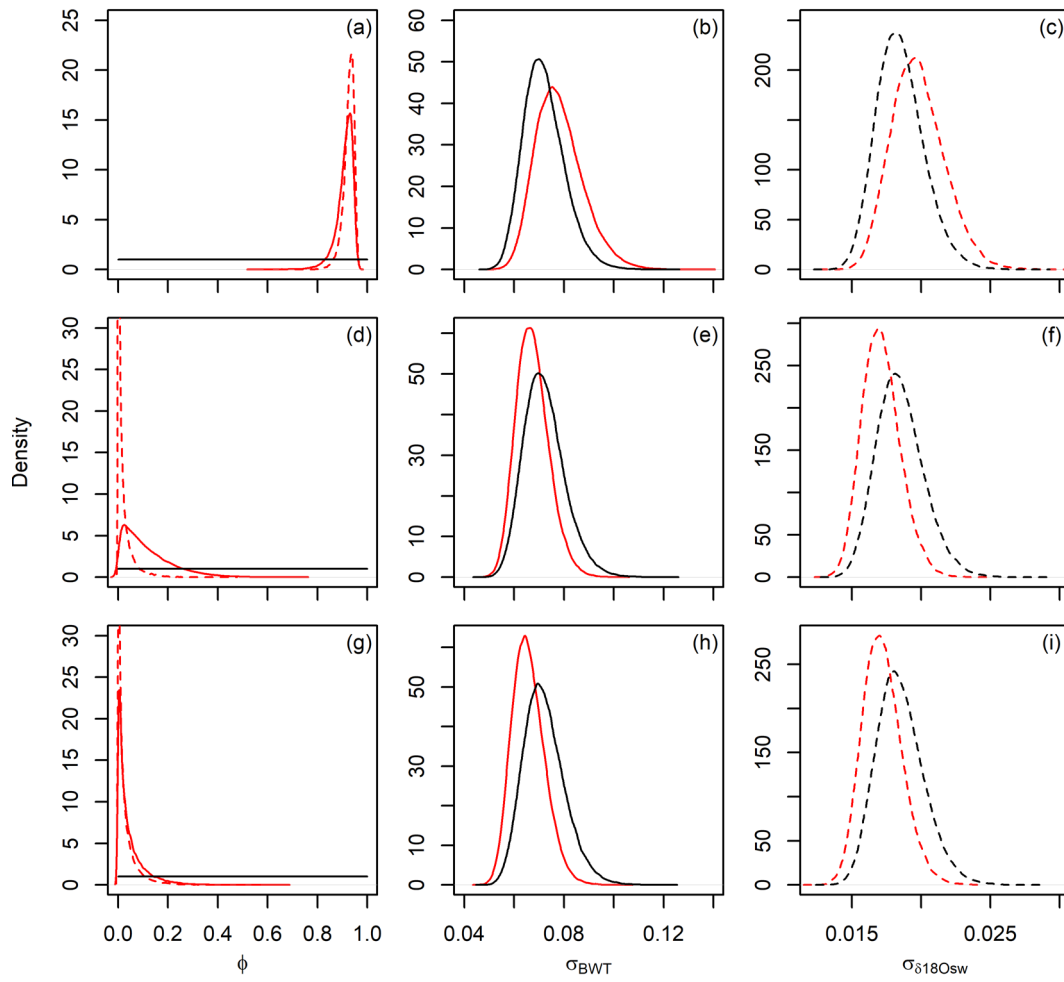
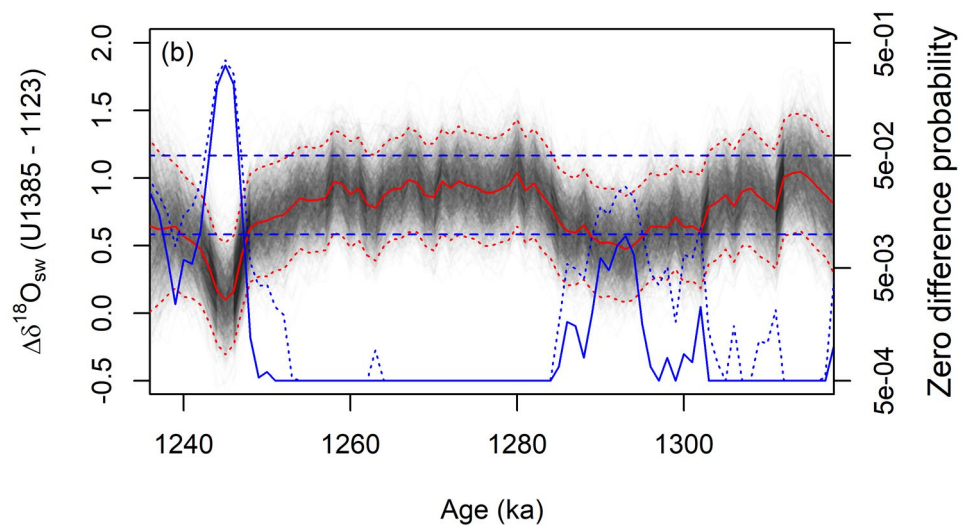
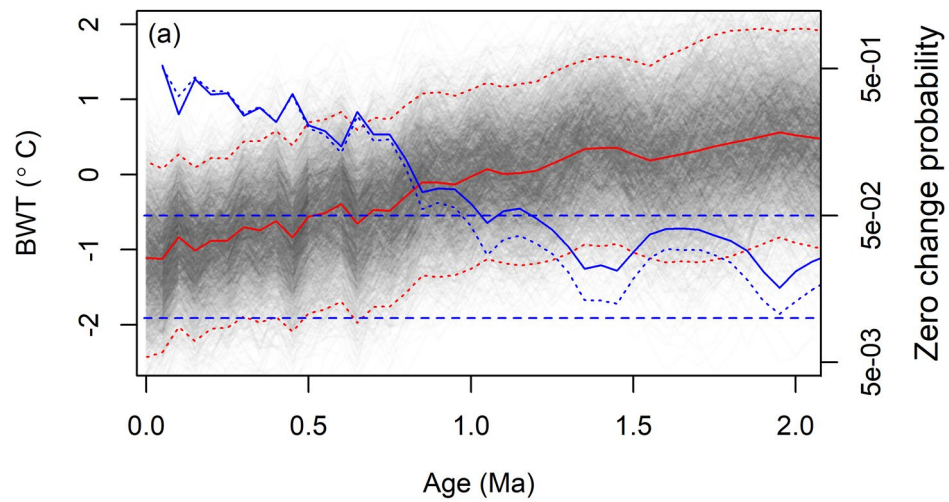


Figure 7: Prior (black) and posterior (red) parameter distributions for bottom water temperature (*BWT*, solid) and seawater  $\delta^{18}\text{O}$  ( $\delta^{18}\text{O}_{\text{sw}}$ , dashed) time series models. (a-c) Site 806. (d-f) Site U1385. (g-i) Site 1123. (a, d, and g) Error autocorrelation (models for both variable used the same prior in a given analysis, shown here in solid black), (b, e, and h) standard deviation of *BWT* error term, and (c, f, and i) standard deviation of  $\delta^{18}\text{O}_{\text{sw}}$  error term.



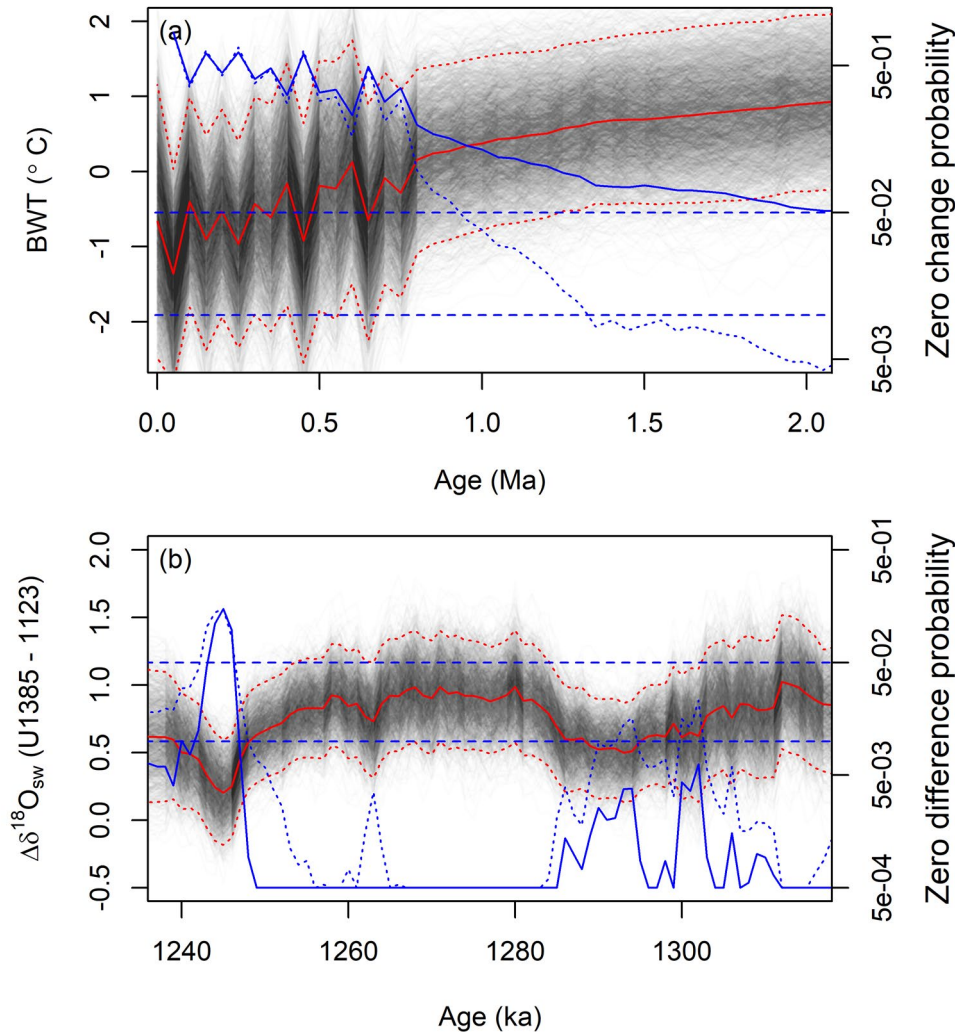


Figure 8: Evaluating changes within and between environmental reconstructions using JPI output. (a) Site 809 bottom water temperature reconstruction from ~2 Ma to present, and probability of no significant change in temperature relative to modern. Grey and red lines show the BWT record. The blue solid ~~and dotted lines show line~~ shows the JPI-estimated probability of no change relative to modern, calculated as the probability of a zero change value at each time step  $t$  given the posterior distribution  $BWT(t) - BWT(0)$  values. The blue dotted line shows an equivalent estimate based on change within (solid) or between (dotted) individual comparisons across posterior samples, calculated as the probability of the modern median value given the posterior distribution of BWT values at time  $t$ . (b) Difference between site U1385 and 1123 seawater  $\delta^{18}\text{O}$  values within individual posterior samples, and probabilities of no significant difference between sites ~~based on comparisons within (solid) or between (dotted) individual posterior samples.~~ Blue solid line shows the probability of a zero difference value given the posterior distribution of differences between the two sites within individual posterior samples. The blue dotted line shows an equivalent estimate based on differences between the two sites calculated from random samples of the single-site analyses. Blue dashed lines in both panels show 5% and 1% probability thresholds; all other symbols as in Fig. 2. See text for details.

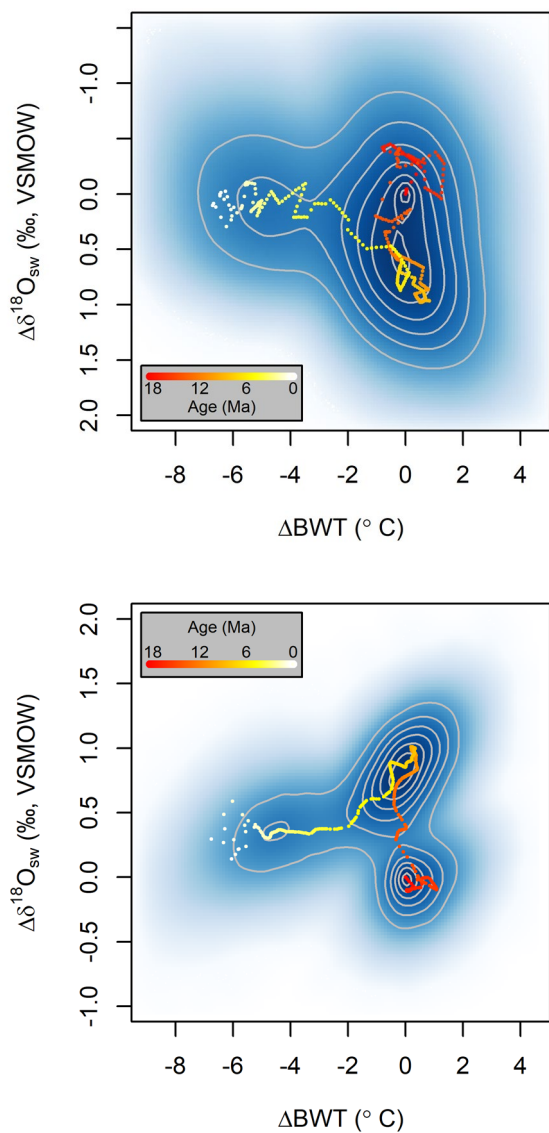


Figure 9: Bivariate density plot of posterior values from the [site 806](#) environmental time series models-(base 50 kyr time steps only). All values are plotted as change relative to 18 Ma within an individual posterior sample. Dots show the median values from the posterior time series.