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Interactive comment on "Sedproxy: a forward model for sediment archived climate proxies" *by* Andrew M. Dolman and Thomas Laepple

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Dear Brett Metcalfe,

We appreciate your taking the time to review our discussion paper and thank you for your constructive and detailed comments that will help to improve the manuscript. We first respond to the main points in your general discussion of the paper and then to the specific comments. We have included portions of your review as blue italicised text.

Response to general discussion.

"The problem with this paper though, is that whilst it is needed by the community the

authors seem to be presenting code that is more a version 0.5 as outlined, throughout the text, by the authors themselves. Throughout the text the authors offer suggestions of 'easy' improvements that they could do to their own code, which is commendable. However, in a couple of instances they note that other code, by other groups, exists that does a similar job and in some parts this weakens the whole."

We do not fully agree with the general characterisation of the sedproxy package as "version 0.5 code". While the processes have been described by other groups (or in previous publications from our group) in nearly all instances, no user-friendly code existed that implements these processes. This is clearly visible in the literature that largely continues to ignore most of the effects. As we describe below, we have added functionality to address your specific points about variable versus static habitat weights and to address proxy calibration uncertainty.

Habitat weightings.

"The authors state that this will help to compare models with proxy data, but if the monthly weighting is static through time can't some-one bypass sedproxy and compare model-March, or a seasonal weighted, output with G. ruber Mg/Ca directly? Likewise, is March really equivalent through time?"

While sedproxy could be bypassed – and a single month or seasonally weighted average from a climate model compared directly to a proxy record – such a comparison would ignore the effects of bioturbation, seasonal biases, aliasing of seasonal and inter-annual variability and measurement error. Therefore, sedproxy which includes these first order effects is a useful tool even with the limitation of static habitat weights, and strongly expands on the classical direct interpretation. However, we also see that the current practise of assuming no seasonality or fixed seasons (e.g. Leduc et al. 2013, Lohmann et al., 2013, Marcott et al. 2013, Shakun et al. 2012) is not optimal. We have therefore extended the model to allow for non-static seasonal-habitat or depth-habitat weights. We have modified the code so that a matrix of weights of the same size as the input climate matrix can be passed in place of a vector of static weights, or a named function plus arguments that will return weights as a function of the input climate. In this way, non-static season/habitat weights can be pre-calculated using either the simple Gaussian response approach of Mix (1987), or something more advanced such as the proposed FAME module (Roche et al 2017). We have ported the relevant functions and data objects from FAME v1.0 Python module (Roche et al 2017) and will include them in the sedproxy R package (under the appropriate GPL license). The calculation of weights from the input climate can be done either within R, or externally with whatever model the user prefers.

Applied to Example 1 from our manuscript, using dynamic habitat weighting from the FAME parametrisation results in an apparent mean temperature change between the glacial (18 ka BP) and the mid-Holocene (5 ka BP) of 1.63 °C, compared to 1.75 °C using static weights derived using PLAFOM with modern day conditions (see Fig. 1). In this example, the difference between static and dynamic weights is small but still illustrates the potential for adaptive behaviour of proxy signal carriers to lead to an underestimation of the magnitude of climate shifts. This effect could be larger for a record from a region with a larger seasonal cycle and/or taxon with a more pronounced seasonality in its productivity. We will expand one of the examples to illustrate the use of dynamic habitat weighting.

Calibration

"The model also uses the same units as the input series, "'we do not explicitly model the encoding process for specific sensors. Other tools have been developed to do this ... and could be used to pre-process the input climate signal'" with the authors suggesting that "'a back-transformation can then be applied to the generated pseudo-proxy records, which itself might model uncertainty by varying the parameters of the

calibration'". My question, why not cut out the middle man in which they risk being supplanted by the code of others and add this into their code? In trace metal geochemistry the calibration(s) of Mg/Ca vs. Temperature is by far one source of error that is overlooked repeatedly. Likewise, the authors should consider who will be their end-user (e.g., whether some end-users may or may not be comfortable with or take the time with pre-processing the data using other code). Therefore, I think the paper could benefit greatly from expansion of the code in ways that the authors themselves list."

We have modified the sedproxy code to add several options for modelling calibration uncertainty. If the argument "proxy.calibration.type" is set to either 'UK37' or 'MgCa', the input climate matrix will be converted using the Uk'37 to temperature calibration from Müller et al (1998), or (one of) the Mg/Ca to temperature calibrations from Anand et al (2003). Alternatively, the input climate matrix and measurement errors can be pre-transformed by the user, the "proxy.calibration.type" is then left at its default value of 'identity'.

Uncertainty in the relationship between temperature and proxy units can be examined by requesting multiple replicate pseudo-proxies. In this case, for each replicate a random set of calibration parameters are drawn from a bivariate normal distribution that represents the uncertainty in the fitted calibration model. The bivariate distributions are parametrised by mean values for the regression coefficients, plus their variance covariance matrices. We have estimated these for the supplied calibrations by refitting regression models to the calibration data used in the original publications (details will be given in a supplement).

Both the Mg/Ca and Uk'37 calibration functions will also accept optional arguments that replace their default parameter values and variance-covariance matrices. For alternative calibration models that have a different functional form, (for these or other proxy types), the name of a user supplied function can be passed that will do the calibration conversion. A template for a user defined function will be given in the documentation.

We have also modified the default plotting functions so that the additional calibration uncertainty is shown.

Response to specific comments:

"(Pg. 3 Line 11-12) "we do not explicitly model the encoding process for specific sensors" maybe explicitly state for clarity that sedproxy doesn't model conversion between temperature and Mg/Ca or Uk37, i.e. calibrations are not used. As it is not clear, as demonstrated by Reviewer 1: "The mathematical formulation of the transformation from Mg/Ca (and UK'37) to temperature is not clear in the text. Which calibration is being used? Can the user input one of their choice?" Perhaps making this clear earlier (on page 3) like you do later at pg 14 line 31 – pg 15 line 5 would benefit the readership."

We have added explicit conversion to and from proxy units, including a method to model uncertainty in this conversion (see above). We will modify the manuscript and documentation accordingly.

"(Pg. 4, Line 10) "We assume here that these effects are minimal" Dissolution is far from minimal, the lysocline is a marked boundary because it is when dissolution becomes apparent (because the rate of dissolution increases) but dissolution is still occurring above the lysocline. Berger suggested that only a small percentage of the flux reaches the seafloor / ends up preserved. If one were to consider it theoretically, productive months (rich in Corg) will likely lead to increased benthic activity and increased CaCO3 dissolution. The authors acknowledge that sedproxy doesn't include a flux component (pg. 15 lines 6-16), if they do add in such a component, it is worth considering that some seafloor processes might also be seasonally driven (or driven by seasonal flux of food/organic matter that can be respired, to the seafloor)."

We will expand the discussion of dissolution in the manuscript text and highlight that this is not modelled and that it may itself have a seasonally driven component.

"(Pg. 4 Line 16) "Due to bioturbation these individuals will be a mixed sample that integrate the climate signal over an extended time period" I would disagree that this is solely a function of bioturbation, low sedimentation rate (e.g. 1 cm per kyr) means that individuals are from potentially any point within 1000 years irrespective of benthic seafloor processes. Perhaps mention here, that low SAR is already a 'smoothed'-integrated record regardless of bioturbation."

The function to calculate bioturbation weights does take into account the width of the sediment layer from which a sample of forams is picked, or Uk'37 extracted (argument "layer.width"). Specifically, it is a convolution with a uniform probability density function (PDF) and the exponential PDF generated by the bioturbation. We will make this detail clearer in the text.

"(Pg. 7 Section 3.3) It would benefit the reader, and add clarity, if the authors better express this section so that sedproxy doesn't become a black box. The independent error term for each proxy type, am I correct in assuming that this is the same as: (Laepple and Huybers 2013; Section 5. Application of the correction filter) "each record requires estimating the two adjustable parameters that define the background variability: the spectral slope (beta) and the standard deviation associated with (eta). We perform an exhaustive search over the values of beta = (0, 0.1,...1.9, 2.0) and STD(eta) = (0, 0.05,...1.95, 2.0), searching for the pair of values that minimize the mean square deviation between the logarithm of the observed spectra and logarithm of the model spectra." later on in the same 2013 paper stating "and a 0.25 and 0.45 standard deviation of eta is prescribed for Uk37 and Mg/Ca respectively". I think, within the text of this paper, the authors need to justify the value of the standard deviation of their Gaussian random variable, how it is constructed for each proxy, its limitation etc. As this will essentially create a model-specific result."

We agree that we should have been clearer about the parametrisation we used for the independent error term. The value of the independent error term is something that the user should decide and justify for a given study. However, as we give suggested values in the manuscript and documentation it is likely that these will be used as "defaults".

It was apparent from the work in Laepple and Huybers 2013 that even after accounting for aliasing and measurement error, there was additional unaccounted independent error in Mg/Ca and Uk'37 proxy records. The magnitude of this error was estimated by tuning a noise parameter to obtain the best fit between power spectra for proxy and pseudo-proxy records. Further, it was shown that these empirically derived parameters were consistent with independent estimates from replicate measurements of Mg/Ca and Uk37. Most datasets contributing to Laepple and Huybers 2013 were based on a similar number of foram tests. Thus a single parameter was a valid approximation even if parts of the true error are to a first order independent of the number of foraminiferal tests (e.g. analytical error) whereas other errors (such as the habitat depth range that was not accounted for in Laepple and Huybers 2013) scale with the sample size.

As sedproxy should be applicable independent of the number of foram tests per sample, we propose to split the independent error term into 2 parts, *sigma.measurement* and *sigma.individual*. *sigma.measurement* will encompass both the analytical error of the measurement process and any other sources of error that are introduced during the preparation of the sample (e.g. cleaning for Mg/Ca). *sigma.individual* will describe all remaining variations, for example inter-individual variations or the depth habitat if unaccounted for. This error will scale with the number of individuals and is likely to be site and species dependent, although the empirical estimates of the sum of both error terms in Laepple and Huybers suggested similar values between study sites. We will describe both error terms and the proposed default values in detail in the revised manuscript.

"(Pg. 10, Line 12) "the input climate signal smoothed to centennial resolution" why have the authors smoothed the input variable? Does this not contradict the point of the model? Furthermore, how was it smoothed, which method? It is only mentioned

here and table 1 (where "block average" smoothing is identified) that there is mention of smoothing in the record, this should be stated within the main text."

The smoothing is only for display purposes as the annual or monthly variance of the input climate signal is typically so much larger than the processed pseudo-proxy (or real proxy reconstruction) that the plots become unreadable. The forward model always works with the full resolution of the input. This is stated in table 1 and we will make it clearer in the figure legends.

"Figure 3 – would it not be better in panel one (input climate) to show the annual minimum or maximum (as a shading)? Your model has a seasonal weighting component therefore the 'full range' should be included, at present the figure at a glance (without reading the caption) appears to show a narrow temperature window. It also makes it difficult to envision the seasonal weighting. Furthermore, might it be prudent to show the measured proxy values of temperature in more than one panel (other than panel 6)? At least plot the forward model and proxy result together in panel 5. Additionally, what is the error on the reconstructed temperature from Mg/Ca?"

We will add the monthly resolution climate information behind the smoothed version in figure 3 panel 1. We will also combine the bioturbated signal and habitat biased signal in one panel (currently panels 2-3) so that the bias is easier to judge. Similarly, the simulated and observed proxy records will be shown together. This will free-up space to also show the calibration uncertainty in an additional panel.

"(Pg. 11 Section: Influence of the number of foraminifera per sample) Is figure 4 only a single run of each n = 1 and n = 30 for G. ruber? If so, would it not be better to produce a figure similar to Figure 5 with replicates. It would/might show that replicates of n = 1 have a larger spread than replicates of n = 30. . . or not."

We like this idea and are testing how best to include this. A candidate figure is included here (Fig. 2).

"(Pg. 13 Section 7) Globorotalia truncatulinoides is a deep dwelling planktonic foraminifera (~500 m), the rationale behind Scussolini et al.'s species selection was that deeper dwellers would exhibit perturbations within the water mass through the movement of Aghulus leakage rings. Therefore, what is the rationale for adding a seasonal component (Pg. 13 Line 14) in waters >500 m that have little seasonality? (see figure 2 in Scussolini and Peeters 2013)"

In response to the comments from Paolo Scussolini (SC1) we will be adjusting the parameters used for this example to be more realistic. This includes a much-reduced seasonal cycle.

"Also and this is just a point of note regarding Figure 7's mean of 45 foraminifera: larger planktonic varieties (such G. truncatulinoides) are generally heavy, most modern mass spectrometers have an upper or lower end in weight, the standard number of foraminifera that constitute 'bulk samples' of heavy foraminifera is 3-5 specimens (i.e. Cleroux et al., 2013 used 10-25 specimens to make four aliquots, x2 for trace metal and x2 for stable isotope geochemistry). Scussolini and Peeters 2013 took a small portion of a large number of shells thus negating this weight limit: "Between 35 and 55 shells for each species were crushed, and a portion of approximately 150 μg of homogenized calcite fragments was used for stable isotope analysis. This approach was adopted to maximize the number of shells involved and therefore the analyses' representativeness of the foraminiferal population". In the past measurements came from samples with more specimens, that is not the case today, so perhaps a mean with fewer specimens would be more fitting?"

We agree that today, many measurements are performed with fewer specimens. However Figure 7 specifically deals with Scussolini et al. 2013. For this study, as long at the sample was well homogenized, using a mean of 45 foraminifera should be the best approximation to their procedure as the Mg/Ca signal from 35-55 individuals should be present in each of the "bulk" data points in their figure 2.

"(Pg. 14 Line 23) "this enables more quantitative comparisons to be made between climate models and proxy data than would classical direct comparison" whilst sedproxy is for the most part better (theoretically) than a simple comparison of proxy data with Mean annual temperature provided by models, does the fact that neither season or depth vary add its own source of error?"

We have updated sedproxy so that varying habitat weights can be used. Not having varying seasonal and depth habitats does not add a source of error, rather it leaves in a source of error that would still be there with a simple model-data comparison.

"(Pg. 15 Line's 32-35) The funnel effect, at least in sediment traps, in which foraminifera deposited may in fact be 'expatriates' does certainly suggest that foraminifera may not have a signal that is directly related to that above the core site. Personally, however if you combine the depth integrated growth (e.g. Wilke et al. 2006 and references therein) with the suggestion in culture of precipitation of calcite on preceding chambers then for the most part the signal preserved within a shell will be overprinted by the final chamber's signal, or a depth weighted function (Roche et al., 2017). Therefore, a model would need only to take into account the distance covered following mortality (settling speed ~1-2 days from surface to sediment)"

It is reassuring to know that sedimented forams provide a relatively local signal, however we also deal here with organic proxies which have much greater potential for lateral transport (e.g. Mollenhauer et al. 2003). As this is a general discussion, we would like to keep this qualification.

Technical comments

Pg. 1, Line 21: Remove 'marine', replace with planktonic or pelagic

Agreed.

Pg. 2, Line 13: Would Mix 1987 and/or Mulitza et al., 1997 not be more appropriate references for 'the influence of seasonal recording'

We have added Mix here as it is a good reference for the theory. Mulitza et al. (1997, Planktonic foraminifera as recorders of past surface-water stratification) deals more with the depth rather than seasonal effect so we will place this reference elsewhere.

Pg. 3, Line 21: remove duplicate 'thus'

Agreed.

Pg. 5 line 3: change 'or' to 'including', as vital effects (the potential metabolic effects) are not exclusively inter-individual variation (given the individual life histories of foraminifera found within the sediment and or plankton tow samples.

Agreed.

Pg. 13 Line 9 'choose parameter values resembling this study' but then state further 'these choices are partly arbitrary' We will revise the parameter values for this example following the comments in SC1

Pg. 15 line's 25-27 The scenario envisioned is performed by Lougheed et al. (2017)

Reference added.

Once again, we thank you for your comments,

Andrew Dolman.

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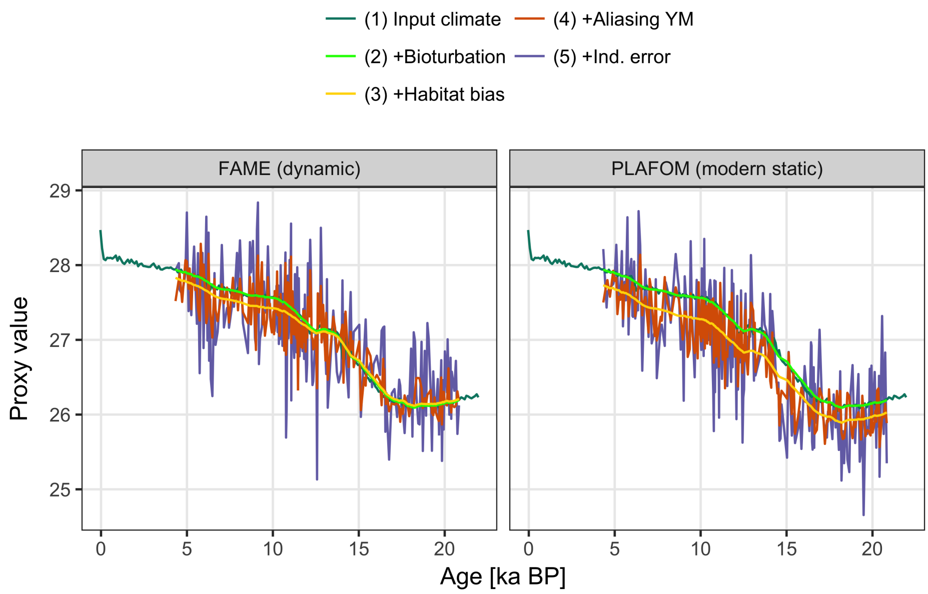

Fig. 1. A comparison of dynamic and static habitat weights.

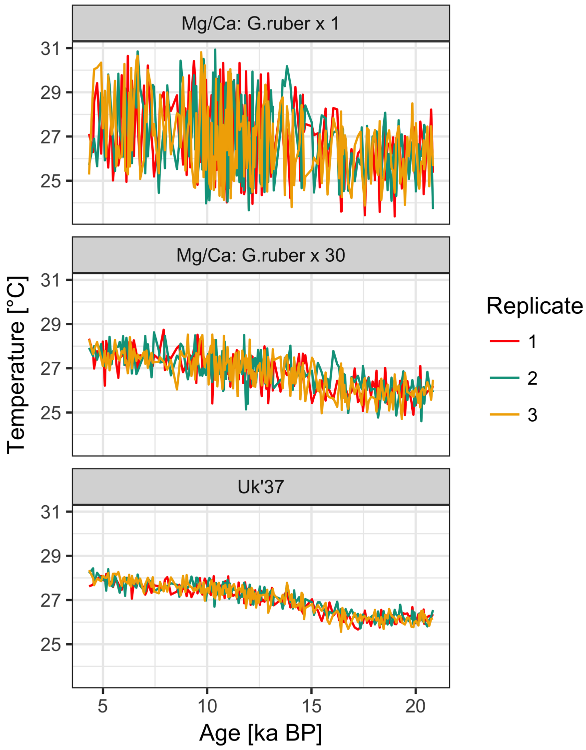

Fig. 2. Replacement for Fig. 4