

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

Andrew M. Dolman and Thomas Laepple

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Dear reviewer,

Thank you for taking the time to review our discussion paper. We thank you for the constructive comments and plan to make several important changes in response to your suggestions. We respond to your comments below and have included relevant portions of the review below (in blue italicised text).

“Do the authors give proper credit to related work and clearly indicate their own new/original contribution? For the most part, yes. Few citations are missing.”

We will check thoroughly for missing citations and add these to the revised version.

C1

“I would suggest the authors add [to the abstract] that sedproxy is an open-source software with open collaboration.”

We will modify the abstract to make clear that sedproxy is open source and that contributions are welcome.

Specific Comments:

“The assumptions that sedproxy makes are presented in the last section of the manuscript. I would suggest moving them upfront to help the reader follow along.”

We will list the assumptions earlier in the “implementation” section (section 3).

“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?”

In the version of sedproxy presented in the discussion paper we did not in fact deal at all with calibration or its uncertainty. We have now modified the code to allow an input climate signal to be converted from temperature to proxy units using either the UK’37 calibration from Müller et al (1998), or (one of) the Mg/Ca to temperature calibrations from Anand et al (2003). Alternatively, the user can supply their own parameter values for the calibration slope and intercept or pre-convert the input climate signal. Uncertainty in the calibration can be examined by applying the calibration using parameters drawn from a bivariate distribution representing the uncertainty in the fitted slope and intercept parameters. We will update the manuscript and package documentation to give examples of this.

“On lines 13-14 (page 3), the authors talk about secondary influences on these proxies but they don’t seem to be take into account in the forward model. One of the advantages of forward modelling is to be able to take into consideration more complex

C2

calibration equations. Why not do this here?"

These kinds of secondary effect could be included with a user-supplied calibration function, but we think it is beyond the scope of this paper to actually suggest more advanced calibrations.

Minor Comments:

"The introduction is often lacking in proper citations. For instance, it's missing a citation on page 1, line 22 about the use of Mg/Ca as a paleo-thermometer or examples of down-core records."

We agree that it would be useful to the reader if more background references are provided and will do a thorough revision of the citations in the manuscript.

"Page 4, lines 10-11: dissolution effects may not be minimal and may be missed during cleaning/processing if SEM images were not taken. See the manuscript by Hertzberg and Schmidt, 2013, EPSL (doi: 10.1016/j.epsl.2013.09.0444). The authors should reword this comment and add this assumption to their list of assumptions and caveats."

We will expand our discussion of the possible effects of dissolution and add this to the assumptions, which will also be listed earlier in the manuscript.

"Move the discussion about INFAUNAL from section 8 to section 7."

We will discuss INFAUNAL in a revised version of section 7.

Once again we thank you for your comments,

Andrew Dolman.

References.

C3

Anand, P., Elderfield, H. and Conte, M. H.: Calibration of Mg/Ca thermometry in planktonic foraminifera from a sediment trap time series, *Paleoceanography*, 18(2), 1050, doi:10.1029/2002PA000846, 2003.

Müller, P. J., Kirst, G., Ruhland, G., von Storch, I. and Rosell-Melé, A.: Calibration of the alkenone paleotemperature index U37K' based on core-tops from the eastern South Atlantic and the global ocean (60 N-60 S), *Geochim. Cosmochim. Acta*, 62(10), 1757–1772, doi:10.1016/S0016-7037(98)00097-0, 1998.

Interactive comment on *Clim. Past Discuss.*, <https://doi.org/10.5194/cp-2018-13>, 2018.

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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

C1

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

C2

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

C3

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 UK37 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 UK37 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.

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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.

C5

"(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: (Laepplé 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

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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

C7

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).

C8

"(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 as 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.

C9

"(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.

C10

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.

References

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Anand, P., Elderfield, H. and Conte, M. H.: Calibration of Mg/Ca thermometry in planktonic foraminifera from a sediment trap time series, *Paleoceanography*, 18(2), 1050, doi:10.1029/2002PA000846, 2003.

Laepple, T. and Huybers, P.: Reconciling discrepancies between Uk37 and Mg/Ca reconstructions of Holocene marine temperature variability, *Earth and Planetary Science Letters*, 375, 418–429, doi:10.1016/j.epsl.2013.06.006, 2013.

Leduc, G., Sachs, J. P., Kawka, O. E. and Schneider, R. R.: Holocene changes in eastern equatorial Atlantic salinity as estimated by water isotopologues, *Earth and Planetary Science Letters*, 362, 151–162, doi:10.1016/j.epsl.2012.12.003, 2013.

Lohmann, G., Pfeiffer, M., Laepple, T., Leduc, G. and Kim, J.-H.: A model–data comparison of the Holocene global sea surface temperature evolution, *Clim. Past*, 9(4), 1807–1839, doi:10.5194/cp-9-1807-2013, 2013.

Lougheed, B. C., Metcalfe, B., Ninnemann, U. S. and Wacker, L.: Moving beyond the age–depth model paradigm in deep sea palaeoclimate archives: dual radiocarbon and stable isotope analysis on single foraminifera, *Clim. Past Discuss.*, 2017, 1–16, doi:10.5194/cp-2017-119, 2017.

Marcott, S. A., Shakun, J. D., Clark, P. U. and Mix, A. C.: A Reconstruction of Regional and Global Temperature for the Past 11,300 Years, *Science*, 339(6124), 1198–1201, doi:10.1126/science.1228026, 2013.

Mix, A.: The oxygen-isotope record of glaciation, in North America and adjacent oceans during the last deglaciation., vol. K-3, pp. 111–135, Geological Society of America., 1987.

Mollenhauer, G., Eglinton, T. I., Ohkouchi, N., Schneider, R. R., Müller, P. J., Grootes, P. M. and Rullkötter, J.: Asynchronous alkenone and foraminifera records from the Benguela Upwelling System, *Geochimica et Cosmochimica Acta*, 67(12), 2157–2171, doi:10.1016/S0016-7037(03)00168-6, 2003.

C12

Mulitza, S., Dürkoop, A., Hale, W., Wefer, G. and Niebler, H. S.: Planktonic foraminifera as recorders of past surface-water stratification, *Geology*, 25(4), 335–338, doi:10.1130/0091-7613(1997)025<0335:PFAROP>2.3.CO;2, 1997.

Müller, P. J., Kirst, G., Ruhland, G., von Storch, I. and Rosell-Melé, A.: Calibration of the alkenone paleotemperature index U37K' based on core-tops from the eastern South Atlantic and the global ocean (60 N-60 S), *Geochim. Cosmochim. Acta*, 62(10), 1757–1772, doi:10.1016/S0016-7037(98)00097-0, 1998.

Roche, D. M., Waelbroeck, C., Metcalfe, B. and Caley, T.: FAME (v1.0): a simple module to simulate the effect of planktonic foraminifer species-specific habitat on their oxygen isotopic content, *Geosci. Model Dev. Discuss.*, 2017, 1–22, doi:10.5194/gmd-2017-251, 2017.

Scussolini, P., van Sebille, E. and Durgadoo, J. V.: Paleo Agulhas rings enter the subtropical gyre during the penultimate deglaciation, *Climate of the Past*, 9(6), 2631–2639, doi:10.5194/cp-9-2631-2013, 2013.

Shakun, J. D., Clark, P. U., He, F., Marcott, S. A., Mix, A. C., Liu, Z., Otto-Bliesner, B., Schmittner, A. and Bard, E.: Global warming preceded by increasing carbon dioxide concentrations during the last deglaciation, *Nature*, 484(7392), 49–54, doi:10.1038/nature10915, 2012.

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C13

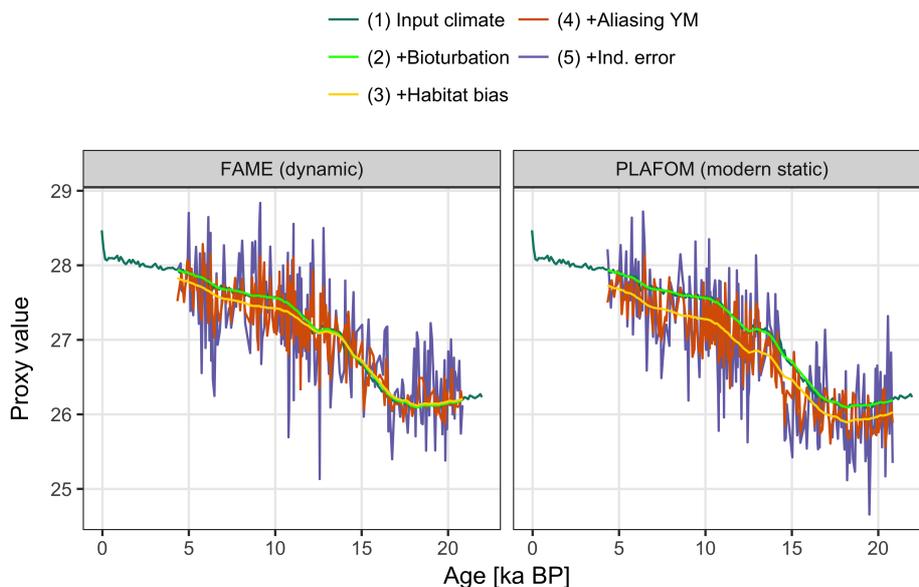


Fig. 1. A comparison of dynamic and static habitat weights.

C14

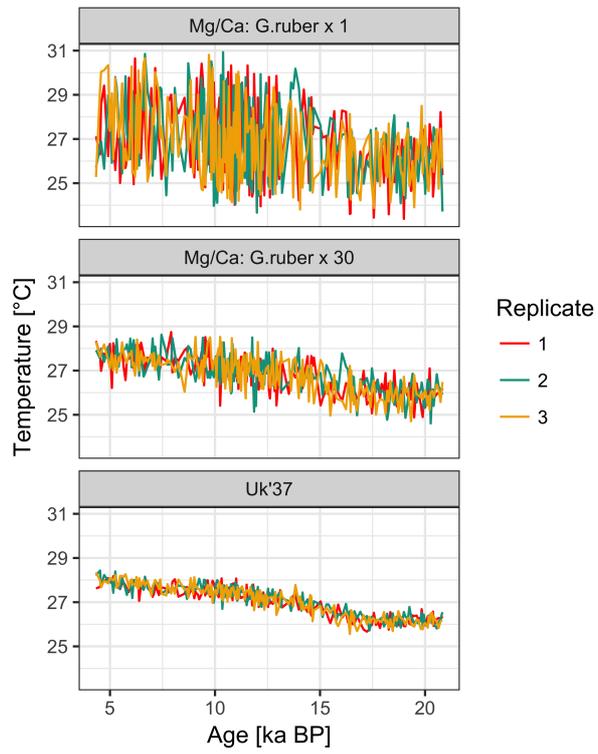


Fig. 2. Replacement for Fig. 4

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Dear Paolo Scussolini,

Thank you for taking the time to read and comment on our discussion paper. We appreciate that in using your study as an example we should have made more effort to justify our choice of parameter values and to check their realism. Our main aim was to illustrate the capability of the sedproxy to simulate IFA type studies and to explore potential alternative explanations for patterns in paleo data. We should have stressed more clearly that we see bioturbation as an alternative explanation rather than presenting it as the most plausible explanation, which of course will depend heavily on the parametrisation.

C1

Your suggestions will greatly improve the manuscript. Here we respond to your specific points in turn. We have included some relevant text from your comment in blue italicised text.

1. Seasonality of $d^{18}\text{O}$ at 400 m:

“First, Scussolini et al. (2013) analysed the planktic foraminifer Globorotalia truncatulinoides (sinistral coiling variety). This organism calcifies at depths beyond 400 or 600 m, according to the relevant literature and to Scussolini and Peeters (2013, Paleoceanography; doi: 10.1002/palo.20041; see also references therein), who compared values from core-top specimens to modern hydrography. At these depths, at the core site, there is hardly any seasonal variation in temperature and salinity. To assume 0.5 ‰ seasonal noise to mimic the $\delta^{18}\text{O}$ signal seems therefore inappropriate. I expect that this shouldn't change the position or magnitude of the peak in variability simulated by 'sedproxy', but it would be advisable to rectify the calculations to reflect this.”

We accept that there is very little seasonality in $d^{18}\text{O}_{sw}$ at these depths and we have removed seasonality from the calculation. However, we also see that we overlooked the much larger variation in $d^{18}\text{O}$ over the depth habitat of Globorotalia truncatulinoides. Consequently, we have modified this example to demonstrate how the habitat weights can be used with a depth resolved rather than seasonally resolved input climate. We refer to Figure 2 of Scussolini Peeters (2013) to approximate the $d^{18}\text{O}$ depth gradient and use a Gaussian distribution with mean of 520 m and standard deviation of 50 m for the habitat weights.

2. Correction for instrumental variance measured on standards:

“Second, Scussolini et al. (2013) report that they 'corrected the variance of foraminiferal $\delta^{18}\text{O}$ by subtracting that of external calcite standards measured in the

C2

same sequence', with the aspiration to clean their proxy from the spurious effect of measurement noise. It seems that Dolman and Laepple do not take this into account, as they 'assume a measurement noise of 0.1‰ del18O for the IFA and the bulk measurements'."

Unfortunately, our description of the method was too brief as we did in-fact subtract this variance from the IFA variance estimated for the simulation output (line 484 in the supplementary .Rmd file). The effect on our Fig. 8 is however small, as the variance due to measurement error amounts to only 0.01 ‰².

3. Speed of the climate transition:

"Third, Dolman and Laepple assumed 'a climate transition from 0.4 ‰ at 190 ka BP, to 2.6 ‰ at 90 ka BP'. The signal in core 64PE-174P13 goes from ca. 1.6 ‰ at 190 ka BP, to 1.3 ‰ at 90 ka BP (see fig. 2 in Scussolini et al. 2013). Where were the values of 0.4 and 2.6 ‰ taken from? In any case, this choice of such extended time frame is puzzling, as the sharp change in del18O occurs obviously across the glacial termination (ca. 140 to 125 ka BP)."

Regarding the assumed climate transition between MIS 5 and 6, unfortunately the quoted 0.4‰ at 190 ka BP was a typographical error, the actual value used was 1.4‰ (it was correct in the code in Supplement 01). The upper value of 2.6‰ was taken from fig. 2 in Scussolini et al. 2013 as the approximate mean value prior to the transition at around 140 ka BP.

Additionally, we could have described the logistic function more precisely. The end points of the function were set at 190 ka BP (1.4‰ and 90 ka BP (2.6‰ but most of the transition occurs during a much shorter window between about 130 and 135 ka BP. We will improve the description in the revised version.

4. Bioturbation depth:

C3

"Further, assuming bioturbation reaching 10 cm from the top of the sediment will obviously produce a peak in variability in any record across a signal transition such as a glacial termination. While it is unrealistic to think that bioturbation is absent from core 64PE-174P13, Scussolini et al. (2013) advanced multiple lines of reasoning to exclude strong bioturbation in core 64PE-174P13, not least visible laminations in parts of the record (see also the author's response to referee 1, who raised specifically the point of bioturbation: <https://www.clim-past-discuss.net/9/C511/2013/cpd-9-C511-2013.pdf>). An additional argument against the role of bioturbation and in favor of an interpretation of the variability signal as proxy for Agulhas rings comes from Scussolini et al. (2015, Geology, doi: 10.1130/G36238.1). There, a tight coupling is shown between the Agulhas rings proxy with the ice-volume-corrected seawater del18O of G. truncatulinoides, a proxy for the high salinity anomalies that Agulhas rings seem to have introduced at the core location (see below a snapshot of the relevant figure in Scussolini et al. 2015, showing the two proxies). It is important to note that the two proxies are analytically independent of one another. It is not clear from the manuscript whether the authors have reasons to prefer the interpretation of the signal in terms of bioturbation."

We accept this point. The plausibility of bioturbation as an explanation for the variance peak will depend strongly on the bioturbation depth, which is poorly constrained.

We have re-run these simulations using a range of bioturbation depths and using the depth-resolved input climate and habitat weights mention above in place of seasonality. While the peak in variance remains clear down to bioturbation depths as low as 3 cm, the absolute value and width of the variance peak are a little lower than that seen in Fig. 2 of Scussolini et al. 2013 (see Fig.1). At the same time, for bioturbation depths of 3 and 5 cm, the apparent speed of the climate transition is consistent with the sharpness of transition (approximately 8 ka) seen in the bulk record for G. truncatulinoides in Fig. 2. of Scussolini et al. 2013 (see Fig.2). However, for 10 cm of bioturbation the transition is too spread out.

We cannot of course exclude enhanced Agulhas leakage as the source of increased

C4

IFA variance across the MIS 5-6 transition, and as noted there is other evidence for increased leakage such as the tight coupling between the Agulhas rings proxy and the $d^{18}O$ of *G. truncatulinoides*. However, given that bioturbation depths as low as 3 cm still produce a quite visible variance peak we think that bioturbation is at least a plausible mechanism behind some of the change in variance over the MIS 5-6 transition. We will modify the manuscript to improve the description of the simulation, to describe the use of depth rather than seasonal weighting, and to make clear that we see bioturbation as a possible alternative mechanism but that this depends heavily on the parametrisation.

Once again, we thank you for your comments,

Regards,

Andrew Dolman.

Interactive comment on Clim. Past Discuss., <https://doi.org/10.5194/cp-2018-13>, 2018.

C5

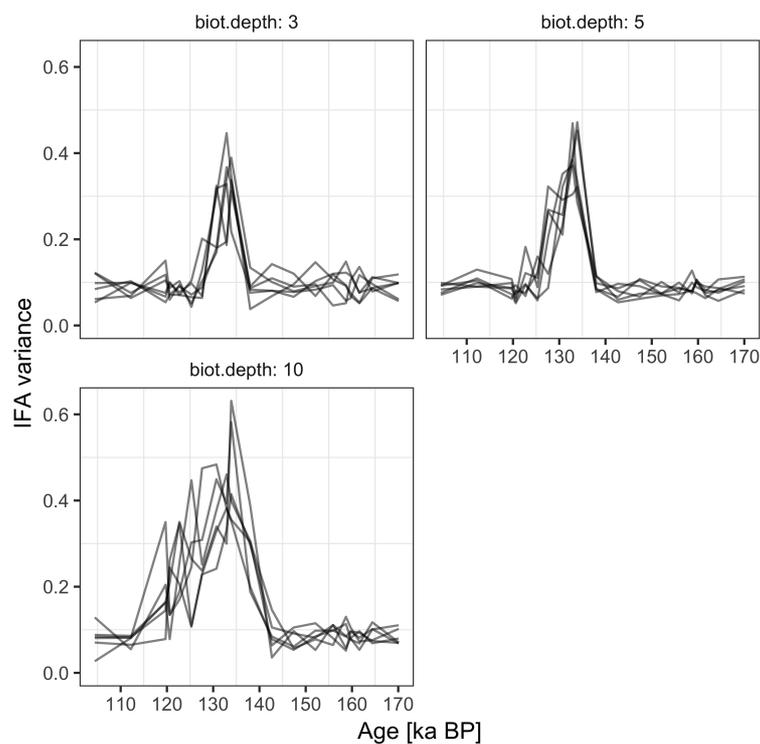


Fig. 1. IFA variance for different bioturbation depths.

C6

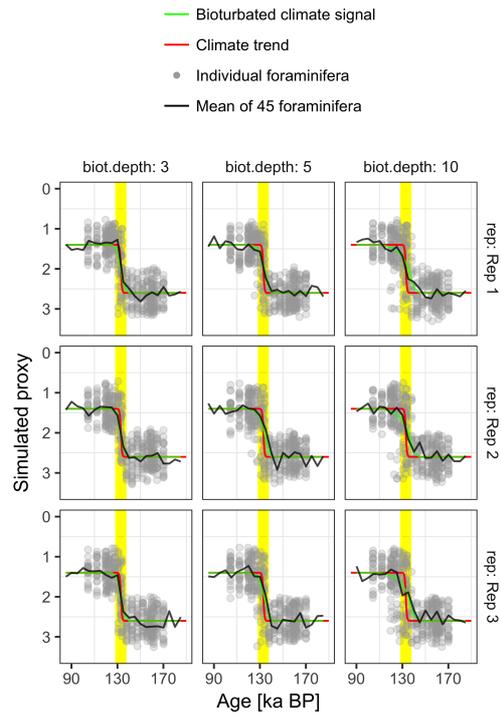


Fig. 2. Simulated bulk and IFA proxies for different bioturbation depths.

Changes made to manuscript.

The major changes to the manuscript are:

- *sedproxy* now includes the ability to use dynamic habitat weights to simulate homeostasis / habitat tracking of the proxy producing organism. The manuscript has been modified to describe this and to remove mention of static weights as a limitation of the model.
- *sedproxy* now includes an explicit sensor model. The input climate is now converted to proxy units, (Mg/Ca or Uk'37), using published calibration functions. The uncertainty in these estimated calibration functions can also be modelled. The manuscript has been modified to describe this.
- The independent error term (previously meas.noise) has been split into two parts representing measurement error and individual error. These are described along with justification for suggested default values.
- The example using IFA has been revised to address the comments by Paolo Scussolini and the two reviewers.
- The “caveats and limitations” section has been removed from the discussion. Those caveats that remain are addressed earlier in the manuscript.

List of changes

1. The abstract now describes *sedproxy* as being open source.
 2. Section 1: Five citations have been added to the Introduction.
 3. Section 2: Description of habitat tracking added.
 4. Section 2.3.1 A clearer explanation that the width of the sediment layer from which proxy carrier material is extracted is taken into account by the model.
 5. Section 3: Description of the input climate matrix is simplified.
 6. Section 3.2: A description of the new calibration / sensor-model has been added.
 7. Section 3.3: The newly implemented dynamic habitat weights are described.
 8. Section 3.3.2: The full expression for calculating the annual weights including the effect of layer width is given here.
 9. Section 3.4: A description of the modified independent error term(s) with suggested default values and justification.
 10. Section 4.1: The first example has been expanded to include an explicit conversion to Mg/Ca units. Associated figures have been modified to address the reviewers' concerns.
 11. Section 4.1.1: A second part to example 1 has been added to show the use of dynamic habitat weights.
 12. Section 4.2: The figure for example 2 now shows the results of 3 replicate pseudo-proxies.
 13. Section 4.4: Example 4, concerning individual foraminiferal analysis, has been thoroughly revised.
 14. Section 5: The discussion has been revised to reflect the changes to the model and the remaining caveats and limitations have been integrated earlier in the manuscript.
- Numerous small changes to the text to improve clarity and readability are not listed here but can be seen in the marked up version of the manuscript.

Sedproxy: a forward model for sediment archived climate proxies

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Abstract. Climate reconstructions based on proxy records recovered from marine sediments, such as alkenone records or geochemical parameters measured on foraminifera, play an important role in our understanding of the climate system. They provide information about the state of the ocean ranging back hundreds to millions of years and form the backbone of paleo-oceanography.

5 However, there are many sources of uncertainty associated with the signal recovered from sediment archived proxies. These include seasonal or depth habitat biases in the recorded signal, a frequency dependent reduction in the amplitude of the recorded signal due to bioturbation of the sediment, aliasing of high frequency climate variation onto a nominally annual, decadal or centennial resolution signal, and additional sample processing and measurement error introduced when the proxy signal is recovered.

10 Here we present a forward model for sediment archived proxies that jointly models the above processes, so that the magnitude of their separate and combined effects can be investigated.

Applications include the interpretation and analysis of uncertainty in existing proxy records, parameter sensitivity analysis to optimize future studies, and the generation of pseudo-proxy records that can be used to test reconstruction methods. We provide examples, such as the simulation of individual foraminifera records, that demonstrate the usefulness of the forward model for paleoclimate studies. The model is implemented as ~~a user-friendly an open-source~~ R package, *sedproxy*, ~~the use of which we hope to which we welcome collaborative contributions. We hope that use of *sedproxy*~~ will contribute to a better understanding of both the limitations and potential of marine sediment proxies to inform about past climate.

1 Introduction

Climate proxies are an imperfect record of the earth's past climate. Climate variations are encoded by geo- or bio-chemical processes into a medium which survives, archived, until it is sampled and the physical or chemical signal decoded back into estimates of direct climate variables. For example, the ratio of magnesium to calcium in the shells (tests) of ~~marine~~ foraminifera varies with the water temperature at which they calcify and thus encodes a temperature signal (Nürnberg et al., 1996). Upon death, these shells (the carrier) ~~sink to the ocean floor and~~ become buried (archived) in the sediment. They can later be recovered from sediment cores and their Mg/Ca ratio measured. Using the modern day relationship between foraminiferal Mg/Ca and temperature, down-core variations in the Mg/Ca ratio in foraminiferal tests can then be decoded back into an estimate of temperature variations back in time (Anand et al., 2003; Elderfield and Ganssen, 2000; Barker et al., 2005).

The climate signal is distorted and obscured at many points during the encoding, archiving and subsequent reading of a climate proxy, and these diverse sources of noise and error need to be taken into account when estimating the true past climate from proxy records. One way to develop, test, and improve our ability to reconstruct climate from proxies is to create mechanistic forward models. These models attempt to simulate the key processes on the entire path from the climate signal to the reconstructed climate: from the encoding of the signal, its archiving in e.g. ice, sediments, wood or coral, recovery of the archived material, cleaning and processing of samples, measurement of the physical or chemical proxy, and its conversion back into units of climate variables such as temperature. Models that attempt to cover this entire process are known as proxy system models (PSMs) (Evans et al., 2013) and detailed PSMs have recently been proposed and implemented for oxygen isotope proxies archived in ice, trees, ~~speleotherms~~ speleothems and corals (Dee et al., 2015).

Climate proxies recovered from sediment cores are widely used to reconstruct past climate evolution on time-scales from centuries (Black et al., 2007) up to millions of years (Zachos et al., 2001). Several processes affecting the climate signal during recording, recovery and measurement have been described in the literature and analysed in specific studies. Examples include the influence of seasonal recording (Schneider et al., 2010; Leduc et al., 2010; Lohmann et al., 2013), the effect of bioturbation (Berger and Heath, 1968; Goreau, 1980), the sample size of foraminifera (Killingley et al., 1981; Schiffelbein and Hills, 1984) ~~and~~, measurement uncertainty (Greaves et al., 2008; Rosell-Melé et al., 2001), and inter-test variability (Sadekov et al., 2008). Despite this body of knowledge, in practice these processes are often considered only in isolation, or not at all, when marine proxy records are interpreted, or when model-data comparisons are made.

The R package *sedproxy* provides a forward model for sediment archived climate proxies so that the above processes can be considered during study design, the interpretation of marine proxy records and when comparing models with data. *sedproxy* is based on and expands the model described and used by Laepple and Huybers 2013 to explain differences in variance between alkenone (Uk'37) and Mg/Ca based climate reconstructions. We first give an overview of the ~~aspects of proxy creation that stages of sedimentary proxy record creation and then describe how these are implemented in~~ *sedproxy* ~~can simulate~~. We then demonstrate how to use the package with a diverse series of use-cases. The source code for the specific version of *sedproxy* used to generate the examples used in this paper is contained in supplement S2, and the latest version of the code and R package are available on Bitbucket <https://bitbucket.org/ecus/sedproxy>.

2 ~~Sediment~~ Creation of sediment archived proxy creation records

The creation of a proxy climate record can be thought of as having three stages: sensor, archive and observation (Evans et al., 2013). Here we describe, for sediment archived proxy records, the key processes that occur in each of these stages and outline which of these are included in *sedproxy*.

2.1 Sensor stage

In the context of a climate proxy, a sensor is a physical, biological or chemical process that is sensitive to climate (e.g. temperature), and creates a measurable record of the climate signal. For example, the widths of tree growth rings are sensitive

to temperature and water availability and are preserved in tree trunks (Evans et al., 2013)(Douglass, 1919). Our forward model can be used for any proxy sensor that records water conditions and is then deposited and archived in the sediment. We consider here, as examples, two climate sensors: the Mg/Ca ratio in the tests of foraminifera, and the alkenone unsaturation index (Uk'37). Foraminifera are single celled protozoa that exude a calcite shell (test) in which a certain proportion of the calcium ions are substituted for magnesium. The ratio of Mg to Ca ions is dependent on the ambient temperature during the process of calcite formation, and thus the Mg/Ca ratio in foraminiferal tests acts as a proxy for temperature during their creation (Nürnberg et al., 1996). Similarly, alkenones are a class of large organic molecules synthesised by some Haptophyte phytoplankton species. The proportion of unsaturated carbon to carbon bonds in the synthesised molecules is temperature dependent and thus the relative unsaturation of alkenone molecules found in sediments can be used as a proxy for temperature (Prahl and Wakeham, 1987). Secondary effects such as the effect of salinity on the Mg/Ca of foraminifera (Hönisch et al., 2013), or nutrient availability on the Uk'37 recorded by the alkenone producers (Conte et al., 1998), might further effect the recorded proxy signal.

~~So as to be applicable to a wide range of climate sensor types, we do not explicitly model the encoding process for specific sensors. Other tools have been developed that do this, e.g. FIRM for foraminiferal $\delta^{18}\text{O}$ (Fraass and Lowery, 2017), and could be used to pre-process the input climate signal. Rather we include a general method for adding error due to uncertainty in the estimated proxy calibration.~~

2.1.1 Seasonal and habitat bias in the sensor

One source of uncertainty common to most climate proxies is a bias towards recording the climate during periods of the year when the proxy generating process is most active (Mix, 1987). Both the foraminifera and the alkenone producing haptophytes have growth rates, abundances and rates of export to the sediment that vary predictably throughout the year (Jonkers and Kučera, 2015; Leduc et al., 2010; Uitz et al., 2010), and hence bias these proxies towards recording the climate during their respective periods of peak production and export. Furthermore, the proxy creating organisms do not necessarily live at and record the surface of the ocean. The producers of alkenones are restricted to the photic zone and thus are ~~thus~~ close to the surface. ~~However;~~ however, for foraminifera, the preferred habitat depth and the depth at which their shells calcify is strongly species dependent and can vary from being close to the surface, to the thermocline or deeper (Fairbanks and Wiebe, 1980; Kretschmer et al., 2017). Therefore, the recorded temperature will not necessarily reflect the sea surface temperature (Jonkers and Kučera, 2017). Whether or not these biases represents an error will depend on how the resulting proxy record is interpreted. However, even when a proxy is interpreted as representing a particular season or depth habitat, the season and depth that a given proxy represents will rarely be known with certainty. Furthermore, it is likely that the seasonal and depth habitat preferences of proxy producing organisms will respond to changes in the climate, i.e. they will show homeostasis or habitat tracking (Mix, 1987; Jonkers and Kučera, 2017) which will likely damp the climate variations in proxy records (Fraile et al., 2009).

2.2 Archive stage

After the creation of proxy carriers such as foraminiferal shells or alkenone molecules, a proportion of these are exported to and buried in the sediment. ~~We assume here that this process is local and ignore the potential for lateral transport of the proxy material in the water column or at the sediment surface.~~

5 2.2.1 Bioturbation

The upper few centimetres of marine sediments are typically mixed by burrowing organisms down to a depth of around 2-15 cm (Boudreau, 1998, 9.8 ± 4.5 cm (1 SD)) (Teal et al., 2010; Trauth et al., 1997, 8.37 ± 6.19 cm), although laminated sediments absent of bioturbation do exist. Marine sediment accumulation rates vary over many orders of magnitude (Sadler, 1999; Sommerfield, 2006) but rates at core locations used for climate reconstructions are typically of the order 1-100 cm ka⁻¹.

10 Thus, bioturbation can mix and smooth the climate signal over a period of ~~many hundreds of years and has~~ decades to millennia ~~and have~~ a strong effect on the effective temporal resolution that can be recovered from a sediment archived proxy (Anderson, 2001; Goreau, 1980).

Other processes occurring during the archive stage may influence the proxy, for example ~~preferential~~ differential dissolution of Mg/Ca in foraminiferal shells (Barker et al., 2007; Rosenthal and Lohmann, 2002; Mekik et al., 2007) and preferential
15 degradation of Uk'37 (Hoefs et al., 1998; Conte et al., 2006). ~~We assume here that these effect are minimal, or would be spotted during sample processing (e.g. dissolution of Mg/Ca), and the signal is preserved.~~

2.3 Observation stage

2.3.1 Aliasing of inter- and intra-annual climate variation

During the observation phase, samples of sediment are taken at intervals along a core and material is recovered in which the
20 proxy signal has been encoded. For ~~proxies~~ Uk'37 extraction and foraminifera picking, these samples are typically taken from 1-2 cm thick sediment layers. Therefore, even in the absence of bioturbation the proxy record will be smoothed by a time period determined by the sedimentation rate and layer thickness.

2.3.1 Aliasing of inter- and intra-annual climate variation

For proxy signals embedded in the tests of foraminifera, ~~this is typically a relatively small sample of about 10-30 measurements~~
25 are typically made on relatively small samples of about 5-30 individuals. Due to ~~bioturbation~~ both bioturbation and the width of the sampled sediment layer, these individuals will be a mixed sample that integrate the climate signal over an extended time period; however, individual planktonic foraminifera live for a period of only 2-4 weeks (Bijma et al., 1990; Spero, 1998) and hence each encodes climate at an approximately monthly resolution. Therefore, if a measurement is made on a sample containing 30 individuals mixed together from a period of 100 years, the resulting value is a noisy 100-year mean and hence inter-
30 and intra-annual scale climate variation is aliased into the nominally centennial-resolution proxy record (Laepple and Huybers,

2013; Schiffelbein and Hills, 1984). This effect may be particularly strong for high latitude cores where the seasonal temperature cycle is large. However the stronger the seasonal climate cycle, the more likely an organism is to grow preferentially during a specific season (Jonkers and Kučera, 2015), and thus aliasing will be reduced, while seasonal bias is increased. For organic proxies such as Uk'37, samples comprise many thousands of molecules and aliasing is likely a minor issue, although clustering in sediment export and distribution is possible (Wörmer et al., 2014).

2.3.2 Other non-climate variability: inter-individual variation, cleaning/processing and instrumental error.

The measurement of proxy values on material recovered from sediment cores will necessarily involve some amount of error. In particular, foraminiferal tests need to be cleaned prior to Mg/Ca measurements and this is an imprecise process. Too little cleaning risks leaving Mg rich mineral phases (Barker et al., 2003), too much may bias the Mg/Ca downwards. Some cleaning, processing and measurement errors will be independent between samples while others may be correlated, for example due to differences between labs (Greaves et al., 2008). In addition to measurement error, there will also be inter-individual variation between foraminifera in their recording of the same climate signal (Haarmann et al., 2011; Sadekov et al., 2008). For example, test Mg/Ca ratios vary between individual foraminifera even when grown under identical conditions (e.g., Dueñas-Bohórquez et al., 2011). Similar inter-individual variation, or "vital effects", also occur for $\delta^{18}\text{O}$ (Schiffelbein and Hills, 1984) (Duplessy et al., 1970; Sc

~~An additional sampling artefact is created due to the need to pick individual foraminiferal tests, or extract Uk'37, from a slice of a sediment that cannot be infinitely thin. Therefore, even in the absence of bioturbation, this material will cover a time period determined by the sedimentation rate and layer thickness. Foraminifera are typically picked from 1-2 cm thick sediment layers, provided enough individuals can be found~~

3 Implementation

20 Here we give an overview of the model implementation, describing which features of proxy creation can be simulated with *sedproxy*. The essential input data, variables and parameters are listed in Table 1 and described in the following paragraphs. Additional optional function arguments are described in the *sedproxy* package documentation.

4 **Implementation**

3.1 Input climate matrix (clim. signal)

25 *sedproxy* takes as input an assumed "true" climate signal, which may come from a climate model or instrumental readings, and returns a simulated proxy value for each of a set of requested timepoints. ~~Returned values are in the same units as the~~ The input climate signal, ~~which may be either temperature or proxy units. All required parameters and input variables are shown in Table 1, and described in the following paragraphs together with an overview of the model implementation.~~

3.2 Input climate matrix ("clim.signal")

The input climate signal is required at monthly resolution in order to be able to simulate is required as a matrix $C_{y,h}$ where y rows are the years and the h columns resolve the habitats being modelled. For example, to model seasonal biases in the recording process and noise aliased from monthly climate variation. It is useful, in the implementation, to view this climate signal as a years-by-months matrix $C_{y,m}$ where y are the years and m are the, there should be 12 months columns representing 12 months of the year. To include other habitat effects, e.g. foraminiferal depth habitats, this matrix can be extended to have e.g. 12 x z columns, where z is the number of discrete habitats h depths to be included. In this case a depth resolved

$$\begin{pmatrix} C_{y_1,h_1} & C_{y_1,h_2} & \cdots & C_{y_1,h_{12z}} \\ C_{y_2,h_1} & C_{y_2,h_2} & \cdots & C_{y_2,h_{12z}} \\ \vdots & \vdots & \ddots & \vdots \\ C_{y_n,h_1} & C_{y_n,h_2} & \cdots & C_{y_n,h_{12z}} \end{pmatrix}$$

3.2 Sensor-model / calibration

The input climate signal would be required. For simplicity we consider only sea surface signals in the examples presented here. can be converted to proxy units using a transfer function based on an established temperature calibration. If the argument `calibration.type` is set to either 'Uk37' or 'MgCa', the input climate matrix will be converted using the global Uk'37 to temperature calibration from Müller et al. (1998), or the multispecies Mg/Ca to temperature calibrations from Anand et al. (2003), respectively. The argument `calibration` can be used to specify one of the taxon specific calibrations from Anand et al. (2003). If `calibration.type` is left at its default value of 'identity', then no transformation takes place. This gives the option for the input climate matrix to be pre-transformed into any proxy type by the user.

$$\begin{pmatrix} C_{y_1,m_1,h_1} & C_{y_1,m_2,h_1} & \cdots & C_{y_1,m_{12},h_z} \\ C_{y_2,m_1,h_1} & C_{y_2,m_2,h_1} & \cdots & C_{y_2,m_{12},h_z} \\ \vdots & \vdots & \ddots & \vdots \\ C_{y_n,m_1,h_1} & C_{y_n,m_2,h_1} & \cdots & C_{y_n,m_{12},h_z} \end{pmatrix}$$

Uncertainty in the relationship between temperature and proxy units can be modelled by requesting multiple replicate pseudo-proxies. 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 and corresponding variance-covariance matrices. We have estimated these variance-covariance matrices for the supplied calibrations by refitting regression models to the calibration data used in the original publications. Due to small differences in the data sets and methods, our parameter estimates deviated slightly from the published values, but for consistency the mean parameter values are set to the published values.

As *sedproxy* does not explicitly model the differential dissolution of foram tests, nor preferential degradation of Uk'37, the implicit assumption is made that that, where is is used, these effect are either minimal or otherwise corrected for during sample processing (e.g. by exclusion of extensively dissolved foram tests). Where a bias due to differential dissolution can be estimated, this could be corrected for using a custom dissolution-correcting temperature calibration (e.g., Mekik et al., 2007; Rosenthal and Lohmann,

5

Both the Mg/Ca and Uk'37 calibration functions will accept optional arguments that replace their default parameter values and variance-covariance matrices. For alternative calibration models that have a different functional form, the function `ProxyConversion` would need to be modified.

3.3 Weights matrix

10 While conceptually *sedproxy* modifies the climate signal according to a sequence of sensor, archive and observation processes, in practice the value of the simulated proxy at a given timepoint is calculated in a single step as the mean of a weighted sample from the original climate signal, plus some independent error term. For each requested timepoint, a matrix of weights, ~~W~~ $W_{y,h}$, is constructed which determines the ~~region of the original climate signal that will be sampled and the~~ probability of sampling any particular value from the climate matrix.

15 The ~~weights matrix W is~~ elements of the weights matrix $W_{y,h}$ are the product of ~~a column vector of~~ annual weights, w_y , which depend on bioturbation, and ~~a row vector either a vector or matrix~~ of habitat weights, w_{mh} , ~~which depend on the seasonality and potentially the depth habitat of the proxy recording process~~ w_h or $w_{y,h}$, corresponding to "static" or "dynamic" habitat weights respectively. Static weights correspond to habitat preferences (e.g. depth or season) that that do not vary over time with climate. Dynamic weights correspond to season and habitat preferences that change in response to climate - such as

20 might be expected from organisms adapting to changing water temperatures by altering their depth in the water column or the timing of their production.

$$W = \begin{pmatrix} w_{y_1} \\ w_{y_2} \\ \vdots \\ w_{y_n} \end{pmatrix} \begin{pmatrix} w_{m_1 h_1} & w_{m_2 h_1} & \cdots & w_{m_{12} h_z} \end{pmatrix} = \begin{pmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,12z} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,12z} \\ \vdots & \vdots & \ddots & \vdots \\ w_{n,1} & w_{n,2} & \cdots & w_{n,12z} \end{pmatrix}$$

3.3.1 Habitat weights (~~season and depth habitat of proxy production and export~~habitat weights) ("proxy.prod.weights")

25 ~~The Static~~ Static habitat weights, $w_{mh}w_h$, are given by a user defined vector defining the seasonality and potentially the depth habitat of the proxy recording process. It has the same length as the number of columns in the input climate signal. ~~In this case where we use monthly sea surface temperature and ignore depth habitats, the habitat weights vector has 12 values. Currently the season and depth habitat in the recording (but not necessarily the climate) is assumed to be invariant over time~~Dynamic habitat

weights can be specified either by passing a named function that will calculate these weights from the input climate matrix, or by passing a pre-calculated matrix of weights of the same size as the input climate matrix. Non-static habitat weights could be generated using either the simple Gaussian response approach of Mix (1987), or something more advanced such as the proposed FAME module (Roche et al., 2017). *sedproxy* includes an R implementation of the `growth_rate_109` function from the FAME v1.0 Python module (Roche et al., 2017) that can be used to predict habitat weights from water temperatures for several foraminifera taxa. More complex models, such as FORAMCLIM (Lombard et al., 2011) or PLAFOM (Fraile et al., 2008), could also be used outside of R to pre-calculate the weights matrix.

There is considerable potential for lateral transport of proxy carriers, particularly the organic proxies such as Uk'37 (Mollenhauer et al., 2009), potentially also foraminifera (van Sebille et al., 2015), so that proxy material in given sediment core may have come from a different location or be a mixed sample representing an area of ocean of considerable size. Lateral transport of proxy material in the water column or at the sediment surface could be modelled by using an input climate matrix with columns for multiple spatial locations, and habitat weights representing the probability that material was transported from a given location.

3.3.2 Annual weights (bioturbation)

For simplicity, *sedproxy* assumes complete mixing within the bioturbated layer, a constant sedimentation rate in the region of each sampled timepoint, and a constant concentration of the proxy carrying material. Under these assumptions, the origin (pre-bioturbation) of material recovered from a given focal depth is described by the impulse response function Eq. (4) (Berger and Heath, 1968). This function is equivalent to an exponential probability density function, with mean equal to the focal depth and standard deviation equal to the bioturbation depth divided by the sedimentation rate. The value of a proxy measured on material recovered from a given depth can thus be viewed as a weighted mean of material originally deposited over a range of depths, with weights given by Eq. (4) (Fig. 4-1). By assuming a locally constant sediment accumulation rate, α , around each focal point, and a fixed bioturbation depth, δ , the bioturbation function can be expressed in units of time rather than space/depth.

In this model, the probability that a particle found at a given focal depth was mixed down from a distance greater than the bioturbation depth, δ , is zero. Theoretically, particles can have been brought up from any distance below the focal depth, but for computational reasons the annual weights vector is restricted to a distance of three bioturbation depths below the focal horizon; this region contains 99% of the mass of the impulse response function. ~~By assuming a locally constant sediment accumulation rate, α , around each focal point, and a fixed bioturbation depth, δ , the bioturbation function can be expressed in units of time rather than space/depth.~~

$$wy_t = \begin{cases} \frac{\alpha \cdot e^{\lambda y_f - \lambda y_t - 1}}{\delta} & y_t - y_f + \frac{\delta}{\alpha} \geq 0 \\ 0 & y_t - y_f + \frac{\delta}{\alpha} < 0 \end{cases} \quad (1)$$

where:

α = sediment accumulation rate in cm a^{-1}

δ = bioturbation depth in cm

$$\lambda = \frac{\alpha}{\delta}$$

y_f = the focal year, and

$$x = y_t - y_f + \frac{\delta}{\alpha}$$

To account for the fact that foraminiferal tests are collected, or Uk'37 extracted, from a layer of sediment of a certain thickness (layer.width layer.width). The bioturbation function is convolved with a uniform probability density function with a width equal to the layer thickness (Eq. 2). The effect of layer.width is small unless the bioturbation depth is small relative to the layer width.

$$wy_t = \begin{cases} 0 & z < -L \\ \frac{e^{-\lambda L - \lambda z} \cdot (e^{\lambda L + \lambda z} - 1)}{2L} & -L \leq z \leq L \\ \frac{(e^{2\lambda L} - 1) \cdot e^{-\lambda L - \lambda z}}{2L} & z > L \end{cases} \quad (2)$$

where:

$$z = y_t - y_f + \frac{\delta}{\alpha}$$

$$L = \text{layer.width}/2$$

While the assumption of complete mixing with a sharp cutoff is unlikely to be true, the general effects of bioturbation should also apply under conditions of incomplete mixing and the code could be modified to use a more complex bioturbation model (e.g., Guinasso and Schink, 1975; Steiner et al., 2016). However, when sedimentation rates are low relative to mixing rates, more complex mixing models converge to the simple box type model that employed here (Matisoff, 1982). *sedproxy* further assumes a constant bioturbation depth over time, as the bioturbation depth is generally not known for each setting and cannot easily be reconstructed down-core. Bioturbation depth may be related to productivity and sedimentation rate, but its predictability for a given core seems to be low (Trauth et al., 1997). The recent development of radiocarbon measurements on small samples (Wacker et al., 2010) might allow the extent of bioturbation to be constrained using replicate measurements from individual depth layers (e.g. Loughheed et al., 2017) and such information could be included in *sedproxy* in the future.

3.3.3 Summing or sampling

For proxies such as foraminiferal Mg/Ca, where typically a small number of foraminiferal tests ($\sim 30N$) are cleaned and measured for each depth/timepoint in a sediment core, the proxy at time t , Pr_t , is the mean of a random sample of N elements of the input climate matrix C , with the probability that a particular element is sampled given by the weights matrix W , plus some independent error term ε (Eq. 3).

$$Pr_t = \frac{1}{N} \sum_{i=1}^{i=N} \{C^{(i)}, W^{(i)}\} + \varepsilon \quad (3)$$

For proxies such as Uk'37, it is assumed that there are effectively infinite samples taken for each timepoint at which the proxy is evaluated. In this case the proxy at time y Pr_t is the sum of the element-wise product of the climate and weights matrices - (Eq. 4).

$$Pr_t = \sum (C \circ W) + \varepsilon \quad (4)$$

5 3.4 Independent error term ("meas.noise" sigma.meas, sigma.ind)

The error term ε is added as an independent Gaussian random variable with mean $\mu = 0$, and standard deviation σ dependent on the proxy type. For foraminiferal Mg. The value of σ is controlled by the parameters `sigma.meas` (σ_{meas}), and `sigma.ind` (σ_{ind}). σ_{meas} describes 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 we use $\sigma = 0.46$, for Ca). σ_{ind} quantifies inter-individual variation for proxies that are measured on samples of discrete individuals such as foraminifera, and its contribution to ε is scaled by the square root of the number of individuals in the sample, N (Eq. 5).

$$\sigma = \sqrt{\sigma_{meas}^2 + \frac{\sigma_{ind}^2}{N}} \quad (5)$$

Appropriate values for these error parameters will depend on the proxy type, and for σ_{ind} in particular they may also be site and species dependent, although the empirical estimates of the sum of both error terms in Laepple and Huybers 2013 suggested similar values between study sites. We propose that σ_{meas} should be set to typical lab values for the reproducibility of measurements on real world material. For Uk'37 we use a value of 0.23°C , which was the mean replicate error of all Uk'37 $\sigma = 0.25$ (Laepple and Huybers, 2013). These errors represent not just instrumental measurement error, which is typically much smaller than the errors quoted here, but also included error introduced during studies used in Laepple and Huybers 2013. For foraminiferal Mg/Ca we use 0.26°C for σ_{meas} , which corresponds to about 0.07 - 0.11 mmol/mol at 20 and 25°C respectively and lies within the typical reported range (Skinner and Elderfield, 2005; Groeneveld et al., 2014).

The value of σ_{ind} is less constrained as it depends on how much of this variation has been explicitly modelled, e.g. the cleaning of foraminiferal tests and other non-climate variability such as the inter-individual variability of via a seasonally and depth resolved input climate signal and habitat weights. We use 2°C for σ_{ind} , as most examples here do not explicitly include depth habitat. This value is similar to the inter-test variability of approximately 1.6°C estimated for fresh *Globigerinoides ruber* samples by Sadekov et al. (2008). Assuming a typical number of 30 foraminifera individuals per sample, these two sources add up to approximately 0.45°C , the mean replicate error across all Mg/Ca in foraminifera studies used in Laepple and Huybers 2013. For Uk'37 we set σ_{ind} to zero as we typically assume an infinite sample size.

$$\varepsilon \sim \mathcal{N}(\mu, \sigma)$$

Values of σ_{meas} and σ_{ind} are entered in units of °C by default, but can be entered in proxy units if `scale.noise` is set to FALSE.

3.5 Replication

Multiple replicate proxy records can be simulated with a single set of parameters. Due to the stochastic sampling of **monthly**
5 **temperatures and habitats and depths**, the random noise **term-terms, and the randomly sampled calibration parameters**, replicates will not be identical. An additional random bias can be added to each replicate simulated proxy record. This bias is drawn from a Gaussian distribution with mean = 0 and a user definable standard deviation ("**meas.bias**"-`meas.bias` defaults to 0). This bias will be constant for all points in a given replicate and can be used to include **additional** uncertainty in the proxy calibration, or inter-lab variation in analytical results.

10 4 Using *sedproxy*

To illustrate the use of *sedproxy* we provide here a number of **simple** examples together with the R code to execute them.

4.1 Example 1: A foraminiferal Mg/Ca pseudo-proxy record for sediment core MD97-2141

In this first example, we demonstrate how to simulate an already measured proxy record as closely as possible. We use the foraminiferal Mg/Ca based temperature reconstruction for sediment core MD97-2141 (Table 2) in the Sulu Sea (Rosenthal
15 et al., 2003).

As an input climate signal we take the monthly sea surface temperature output from the TraCE-21ka "Simulation of Transient Climate Evolution over the last 21,000 years" (Liu et al., 2009), using the grid cell closest to core MD97-2141.

We use an Mg/Ca calibration with user supplied mean values for the slope and intercept set to those used by Rosenthal et al. (2003) which
reduce a bias due to partial dissolution. The seasonality of *Globigerinoides ruber*, the foraminifera for which test Mg/Ca ratios
20 were measured, is taken from the dynamic population model PLAFOM, driven with modern climatology (Fraile et al., 2008) (Fig. [2a2a](#)). Sediment accumulation rates were estimated from the depth and age data associated with core MD97-2141 and provided in the supplemental data to Shakun et al 2012. These data are included in the *sedproxy* R package as example data and are also used in the later examples.

The function `ClimToProxyClim` is used to forward model a proxy record from an assumed climate. We request values
25 of the proxy at the timepoints of the observed proxy. Descriptions of all the the main function arguments can be found in Table [1](#). Or from the 1, other optional arguments are described in the package documentation. From the R console type `?ClimToProxyClim` to see the help page.

```
library(sedproxy)
```

```

# Reverse matrix so that top row is most recent year,
# also convert from Kelvin to °C
N41.t21k.climate.in <- N41.t21k.climate[nrow(N41.t21k.climate):1, ] - 273.15

# Convert matrix to a ts object and set start to most recent year,
# in this case -39 (1989 in years "before" 1950)
N41.t21k.climate.in <- ts(N41.t21k.climate.in, start = -39)

# Set seed of random number generator so that the results are reproducible.
set.seed(20170824)

# Call the forward model
Mg_Ca.cal <- ClimToProxyClim(
  clim.signal = N41.t21k.climate.in,
  timepoints = N41.proxy$Published.age,
  calibration.type = "MgCa",

  # Custom calibration parameters from Rosenthal et al. (2003)
  slp.int.means = c(0.095, log(0.28)),

  sed.acc.rate = N41.proxy$Sed.acc.rate.cm.ka,
  plot.sig.res = 1,
  habitat.weights = N41.G.ruber.seasonality,
  sigma.meas = 0.26, sigma.ind = 2,
  n.samples = 30)

```

In addition to the estimated [final proxy](#) [pseudo-proxy](#) timeseries, *sedproxy* calculates and returns the unobserved intermediate stages of proxy creation to assist in the interpretation of the simulated proxy. We provide a plotting function `PlotPFMs` which will display the output from `ClimToProxyClim`, together with an observed proxy record if this is added to [the](#) plotting data. `PlotPFMs` returns a ggplot object that can be customised using the standard ggplot functions (Wickham, 2009). [For brevity, we show here only code to generate the default figure, complete code for the publication figure is provided as supplementary material.](#)

```

plot.dat <- Mg_Ca.cal$everything

# Rescale timepoints to ka for plotting
plot.dat$timepoints <- plot.dat$timepoints / 1000

# Add observed proxy record
obs.proxy <- data.frame(timepoints = N41.proxy$Published.age / 1000,
                        value = N41.proxy$Proxy.value,
                        stage = "observed.proxy",
                        scale = "Proxy units",
                        replicate = 1)

plot.dat <- rbind(plot.dat, obs.proxy)

PlotPFMs(plot.dat)

```

Fig. 3-3 shows the forward modelled Mg/Ca proxy record for core MD97-2141 (5), together with the input climate signal smoothed to centennial-annual resolution (1), the intermediate stages of proxy creation (2-4), and the observed proxy reconstruction as published in Rosenthal et al. 2003. Although the observed (*) and forward modelled (5) proxy records appear to have similar variance, the simulated bioturbation first removes most features of the input climate signal before the aliasing and noise term increase the variability again. In this example, the median sediment accumulation rate is 25.6 cm ka⁻¹, which, assuming a bioturbation depth of 10 cm, corresponds to an expected standard deviation in the ages of individual foraminifera recovered from a single depth of 390 years. Trends remain visible at temporal resolutions of approximately 2 ka and greater, as does a single-centennial-to-millennial scale feature present in the input climate signal at around 12.5 ka BP.

The combination of the seasonal temperature cycle present in the monthly TraCE-21ka simulation, and the seasonality of *G. ruber* taken from Fraile et al. 2008 PLAFOM (Fraile et al., 2008), shifts the forward modelled proxy by about -0.26 °C (Fig. 3-3, 2-3). This shift varies from -0.29 to -0.16 °C depending on the strength of the seasonal cycle, which changes due to the variations in the orbital parameters.

The single-centennial-to-millennial scale feature still visible in the bioturbated signal at 12.5 ka BP is obscured first by the effects of first obscured by noise due to aliasing of annual and intra-annual variance, dominated by the seasonal climate cycle, onto the proxy record due to relatively small number of foraminifera contributing to each proxy data point. Further measurement error erases any trace of these centennial-to-millennial scale features in the final forward modelled proxy; only multimillennial and greater scale trends remain visible.

The resolution of features that can be seen in the final forward-modelled proxy is consistent with Rosenthal et al. 2003's interpretation of the observed Mg/Ca proxy, from which they estimate the LGM-Holocene temperature increase, but find no

other significant features. However, the features visible in a forward modelled proxy are of course dependent on both the input climate signal - in this case the TraCE-21ka simulation - and parameter values used in the proxy simulation.

5 **Example 2: Influence of the number of foraminifera per sample**

4.0.1 **Example 1b: Dynamic habitat weights**

- 5 To illustrate the use of dynamic habitat weights we compare here the static weights (derived from PLAFOM with modern climatology) with weights computed using the R implementation of the `growth_rate_109` function from the FAME v1.0 Python module (Roche et al., 2017) included in `sedproxy`. For this comparison we run the forward model with an 'identity' calibration, i.e. without converting the input climate to proxy units. All other arguments remain the same.

```
# growth_rate_109_R requires temperatures in Kelvin
wts.fame.R <- growth_rate_109_R("ruber", N41.t21k.climate.in + 273.15)

FAME <- ClimToProxyClim(clim.signal = N41.t21k.climate.in,
                       timepoints = N41.proxy$Published.age,
                       calibration.type = "identity",
                       habitat.weights = wts.fame.R,
                       sed.acc.rate = N41.proxy$Sed.acc.rate.cm.ka,
                       sigma.meas = 0.26, sigma.ind = 2,
                       n.samples = 30)
```

- Using dynamic habitat weighting from the FAME parametrisation results in an apparent mean temperature change between the earliest 2000 years of this record (18-20 ka BP) and the most recent 2000 years (4-6 ka BP) of 1.61 °C, compared to 1.72 °C using static weights derived using PLAFOM with modern day conditions (Fig. 5). 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, also, for comparability with PLAFOM, we used only SST values and not a depth resolved climate, which would offer further potential for habitat tracking. Note that when creating dynamic weights as a function of temperature, care should also be taken to restrict the occurrence of taxa to their known depth ranges.

4.1 **Example 2: Influence of the number of foraminifera per sample**

- To examine the influence of the number of individual foraminifera per timepoint on the uncertainty due to seasonal aliasing, we simulate two artificial Mg/Ca records with 1 and 30 individual foraminifera per sample. For comparison, we also simulate

a Uk'37 record, for which the sample size per timepoint is assumed to be infinite. For simplicity we assume that alkenones are produced uniformly throughout the year.

```
Mg_Ca.1 <- ClimToProxyClim(  
  clim.signal = N41.t21k.climate.in,  
  timepoints = N41.proxy$Published.age,  
  sed.acc.rate = N41.proxy$Sed.acc.rate.cm.ka,  
  habitat.weights = N41.G.ruber.seasonality,  
  sigma.meas = 0.26, sigma.ind = 2,  
  n.samples = 1, n.replicates = 3)  
  
Uk37 <- ClimToProxyClim(  
  clim.signal = N41.t21k.climate.in,  
  timepoints = N41.proxy$Published.age,  
  sed.acc.rate = N41.proxy$Sed.acc.rate.cm.ka,  
  sigma.meas = 0.23,  
  n.samples = Inf, n.replicates = 3)
```

The output from ~~these three runs of the model~~ [three replicate runs with these parametrisations](#) is shown in Fig. 4.6. For brevity, code to generate the figure and perform the simulation with 30 individuals is not shown here but complete code for all 5 examples is provided as supplementary material.

5 ~~Example 3: Correlation between two proxy types.~~

4.1 [Example 3: Correlation between two proxy types.](#)

sedproxy can be used to explore the expected correlation between pairs of proxy records. Here we correlate Mg/Ca and Uk'37 based proxies generated for the same hypothetical sediment core. Records from different locations could be compared by 10 supplying a different input climate matrix for each site.

To emphasise the potential effect of contrasting proxy seasonality on the correlation between two records we use hypothetical seasonal weights. The Uk'37 proxy is again assumed to have a constant production with no seasonality, while production of the Mg/Ca proxy is heavily weighted towards August and September.

We again use the same ~~TRaCE-21ka~~ [TraCE-21ka](#) input climate but for simplicity we use a constant sedimentation rate and 15 request proxy values at equally spaced timepoints. One thousand replicate proxy records are simulated of each type.

```

# 1000 replicates of a hypothetical Uk'37 and Mg/Ca record
Uk37.reps <- ClimToProxyClim(
  clim.signal = N41.t21k.climate.in,
  calibration.type = "Uk37",
  timepoints = seq(100, 21000, by = 1000),
  sed.acc.rate = 25, habitat.weights = rep(1/12, 12),
  sigma.meas = 0.23,
  n.samples = Inf, n.replicates = 1000)

MgCa.reps <- ClimToProxyClim(
  clim.signal = N41.t21k.climate.in,
  calibration.type = "MgCa",
  timepoints = seq(100, 21000, by = 1000),
  sed.acc.rate = 25,
  habitat.weights = c(0, 0, 0, 0, 0, 0, 0, 0.2, 0.7, 1, 0.6, 0, 0),
  sigma.meas = 0.26, sigma.ind = 2,
  n.samples = 30, n.replicates = 1000)

proxies <- bind_rows("Mg/Ca"=MgCa.reps$everything,
                    "Uk'37"=Uk37.reps$everything,
                    .id = "Proxy")

proxies <- filter(proxies, stage %in% c("reconstructed.climate"))

```

The Mg/Ca based artificial records show greater variance than Uk'37 due to a combination of aliasing caused by the finite number of foraminiferal tests and an assumption of higher measurement error (Fig. 57). In addition to a mean offset between the two proxy types, the hypothetical Mg/Ca proxy shows a much stronger glacial-interglacial transition because the effect of the bias towards recording summer climate increases when the amplitude of the seasonal cycle is larger and this was maximal at around 10 ka BP.

Fig. 68 shows the distribution of correlations between replicated pairs of hypothetical Mg/Ca, Uk'37, and Mg/Ca-Uk'37 records, calculated over both the past 10k years (Holocene), and the past 21k years which include the de-glaciation. Over the Holocene, the average correlation between simulated pairs of proxy records is low, even for pairs of the same proxy type. The average correlation between Mg/Ca and Uk'37 proxy records is even negative, due to the simulated warming annual mean temperature, sampled by the Uk'37 record, but slightly cooling summer temperature sampled here by the hypothetical summer growing foraminifera. Similar contrasting trends have been observed between real Mg/Ca and Uk'37 records over the Holocene

(Leduc et al., 2010). Correlations between Uk'37 Uk'37 pairs are slightly higher than those between Mg/Ca pairs, due to the lower measurement noise and lack of aliasing we assume for Uk'37. When the proxy records include a large climate transition, such as the deglaciation between 21ka BP and 10ka BP, correlations between all pairs become high.

5 Example 4: Individual Foraminiferal Analysis

5 4.1 Example 4: Individual Foraminiferal Analysis

In individual foraminiferal analysis (IFA), the population statistics (e.g. standard deviation or range) of proxy values measured on individual foraminifera recovered from the same depth, are used to infer changes in climate variability - such as changes in the El Niño Southern Oscillation (ENSO) system (e.g., Koutavas and Joanides, 2012; Killingley et al., 1981), or changes in the amplitude of the seasonal cycle (e.g., Ganssen et al., 2011; Wit et al., 2010). *sedproxy* can be used to simulate IFA by setting `'n.samples = 1'` and `'n.replicates'` `n.samples = 1 and n.replicates` to the number of individuals measured per timepoint. This approach bears some similarity with INFAUNAL (Thirumalai et al., 2013); however, while INFAUNAL was designed to test the sensitivity of IFA to the seasonal cycle and inter-annual variability, and therefore includes a specific analysis on the simulated IFA distributions, *sedproxy* is more general and also includes the effects of bioturbation and habitat weighting.

15 Motivated by the study from Scussolini et al. 2013, which examined changes in the IFA distribution of $\delta^{18}\text{O}$ during the penultimate deglaciation, we simulate a case study that demonstrates the effect of bioturbation on the IFA distribution ~~and choose parameter values resembling this study. The sedimentation rate is set to 1.3 cm ka^{-1} , we simulate 20 foraminiferal tests for the IFA analysis, 45 foraminiferal tests for the bulk measurements and assume a measurement noise of $0.1 \text{ ‰ } \delta^{18}\text{O}$ for the IFA and the bulk measurements.~~

20 To mimic the reconstructed climate signal of Scussolini et al. (2013) ~~, we assume a~~ we generate an input climate signal in units of $\delta^{18}\text{O}$. We assume a logistic shaped climate transition from 0.4 ~~1.4~~ ‰ at ~~190 131~~ ka BP, to 2.6 ‰ at ~~90~~ ka BP with the shape of a logistic function. Finally, ~~135~~ ka BP. To this signal we add stochastic climate variability following power law scaling with slope = 1 (Laepplé and Huybers, 2014) ~~, and variance 0.15 and sinusoidal seasonal variations with an amplitude of 0.5 and variance = 0.0025 . In this region, the foraminifera *Globorotalia truncatulinoides* (sinistral coiling variety) calcifies at a mean~~
25 depth of approximately 520 m, with a standard deviation of 50 m (Scussolini and Peeters, 2013). We model individual variation arising from this using an input climate matrix with 13 columns representing depths from 370 - 670 m, with $\delta^{18}\text{O}$ anomalies corresponding to the observed $\delta^{18}\text{O}$ gradient of approximately 0.003 ‰ m^{-1} and habitat weights from a Gaussian distribution with mean = 520, SD = 50. The sedimentation rate is set to 1.3 cm ka^{-1} . We run the forward model with bioturbation depths of 3, 5 and 10 cm and simulate 20 foraminiferal tests for the IFA analysis, 45 foraminiferal tests for the bulk measurements. We
30 set measurement noise (`sigma.meas`) to $0.1 \text{ ‰ } \delta^{18}\text{O}$ for the IFA and the bulk measurements and add no additional individual variation (`sigma.ind = 0`). These choices ~~are partly arbitrary but~~ reproduce similar IFA and bulk variance as those shown in ~~Scussolini et al. 2013~~ Scussolini et al. (2013) (Fig. 7)-9). As in Scussolini et al. (2013), for each simulated IFA sample we calculate the variance between individual foraminiferal $\delta^{18}\text{O}$ and subtract the variance due to measurement error.

At the ~~measured-observed~~ sediment accumulation rate of 1.3 cm ka^{-1} and with ~~an-assumed-bioturbation-depth-of-assumed~~ ~~bioturbation depths of 3, 5 or~~ 10 cm, the expected standard deviation in ages of material found at a given depth is approximately ~~7900 years~~. ~~Thus 2300, 3800 and 7700 years respectively.~~ ~~Thus,~~ bioturbation mixes material across the deglaciation, so that samples with a mean age of between 110 and 140 ka BP contain a mixture of glacial and inter-glacial material, and hence show a higher standard deviation in $\delta^{18}\text{O}$, with a peak at around 135 ka BP (Fig. 10). ~~The peak in variance remains clear for bioturbation depths as low as 3 cm, but its absolute value and width are a little lower than that seen in Fig. 2 of Scussolini et al. (2013). At the same time, at bioturbation depths of 3 and 5 cm, the apparent speed of the climate transition is consistent with the sharpness of transition (approximately 8 ka) seen in the bulk record for *G. truncatulinoides*, but for 10 cm of bioturbation the transition is too spread out. The forward modelling exercise therefore indicates that bioturbation is a possible alternative mechanism for the variance peak, but also indicates that the conclusions are sensitive to the parametrisation.~~

Forward modelling cannot disprove enhanced Agulhas leakage as the source of increased IFA variance across the MIS 5-6 transition, and there is other evidence for increased leakage such as the tight coupling between the Agulhas rings proxy and the $\delta^{18}\text{O}$ of *G. truncatulinoides* Scussolini et al. (2015). However, given that bioturbation depths as low as 3 cm still produce a quite visible variance peak we argue that bioturbation is at least a plausible mechanism behind some of the change in variance over the MIS 5-6 transition. ~~This demonstrates that bioturbation can have a significant effect on the IFA distribution in low sedimentation rate settings.~~

5 Discussion and conclusions

We present ~~a the first~~ forward model for the simulation of ~~marine~~ sediment based proxy records from climate data. We ~~choose to~~ include the main well constrained processes affecting sedimentary signals while keeping it general enough to be usable for a large set of problems ~~in paleo-oceanography~~. The *sedproxy* model is implemented as a user-friendly R package in an open-source framework (R Core Team, 2017).

Our forward model ~~combines-relies on~~ and extends the work of many previously published studies and models concerning ~~single processes in~~ the formation of sedimentary records. For example, several prior studies have ~~suggested or~~ investigated the effect of seasonality and/or depth habitat on the recorded proxy signal (e.g., Leduc et al., 2010; Liu et al., 2014; Lohmann et al., 2013; Schneider et al., 2010). ~~In addition to the effect on the signal evolution and trends considered in these studies, sedproxy includes the effect on proxy variability caused by the finite sample size in combination with the habitat range.~~

~~For the specific application of interpreting the variability of individual foraminifera (IFA), our model bears some similarities with INFAUNAL (Thirumalai et al., 2013); however, while INFAUNAL was designed to test the sensitivity of IFA to the seasonal cycle and inter-annual variability, and therefore includes a specific analysis on the simulated IFA distributions, sedproxy is more general and also includes the effects of bioturbation, such as shown in Example 4.~~

~~Several previous studies~~ ~~Others~~ have examined how bioturbation reduces the amplitude of ~~the recorded signal, and recorded signals and,~~ in combination with noise, puts a limit on the temporal resolution of climate events that can be resolved in proxy records (Anderson, 2001; Goreau, 1980); ~~and tools have been developed to model bioturbation (Trauth et al., 1997). While~~

~~being simpler than some of these approaches, the combination in *sedproxy* of bioturbation with the other effects, such as the seasonal aliasing or the measurement error, allows the interaction between these effects to be investigated.~~

~~. Further studies have investigated the effect on the resulting record of sampling a small number of foraminiferal tests (Schiffelbein and Hills, 1984; Thirumalai et al., 2013). By integrating these key features of proxy formation into a single model,~~

- 5 ~~*sedproxy* allows the interactions and combined effect of these processes on the proxy record to be studied for the first time.~~ The relative importance of bioturbation, seasonal biases, aliasing and other noise sources will vary according to the physical characteristics of the sediment core (e.g. sediment accumulation rate), the length of the record, the amplitude of the seasonal cycle, and the amplitude of the signal that is being reconstructed (e.g. a glacial-interglacial transition vs. ENSO). Most importantly, the type of information that is sought from the proxy record will determine whether these processes are important.
- 10 ~~By jointly simulating the major processes affecting the sediment record, *sedproxy* allows these to be considered together.~~

5.1 Applications

sedproxy has many potential applications in paleoclimate research, not limited to those in the examples given above. It can serve as a forward model to create more realistic surrogate records that can be used to test climate field reconstruction methods (e.g., Smerdon et al., 2011) and it can further act as a forward model for inversion based climate reconstructions methods

15 for example using Bayesian hierarchical models (Tingley and Huybers, 2009) or data assimilation schemes (e.g., Klein and Goosse, 2017). Importantly, it allows quantification of the full uncertainty of proxy records related to the processes included in the model. By providing an ensemble of surrogate (pseudo) proxy realizations, rather than single error values, the full temporal structure of the uncertainty can be characterized. Proxy uncertainty can be determined as a function of time-scale, thus separating uncertainties affecting long-term means or time-slices, such as the seasonal recording effects, from temporarily

20 independent noise, such as that caused by aliasing of the seasonal cycle. This enables more quantitative comparisons to be made between climate models and proxy data than would classical direct comparison.

The ability to analyse intermediate stages of the simulated proxy (see example 1) allows the effects of different error sources to be evaluated. Used in this way, *sedproxy* can help optimize and test sampling strategies for sediment cores by evaluating the effect of e.g. the sample thickness, number of foraminifera or analytical uncertainty on the final record. This information can

25 be used to improve the design of studies and to test, prior to a study, whether signals of interest such as centennial scale climate variations could theoretically be resolved by the proxy record.

5.1 Caveats and current limitations

~~While being relatively simple and general, there are inherent caveats to the present forward modelling approach: *sedproxy* does not currently include a complex sensor model – the input climate signal and output proxy signal have the same units, for~~

30 ~~example temperature. While this allows for general application to different proxies archived in marine sediments, it does not account for the uncertainties created during the process of encoding the signal in the proxy material. To overcome this, the input climate signal can be converted to proxy units prior to running the forward model. Any given sensor model could be used, from simple linear or exponential regression to more complex process-based sensor models. 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.

In its current version, *sedproxy* can be used to simulate mean shifts in the recorded climate signal due to seasonality or depth habitat preferences, but not the effects of climate dependent shifts in timing and depth habitat (i.e. habitat tracking, Jonkers and Kučera, 2017) which will likely damp the recorded changes (Fraile et al., 2009). In addition to shifting the seasonal bias in the recorded climate signal, the absolute concentration of the carrier (e.g. foraminifera species) can also change over time in response to climate and this would interact with bioturbation, potentially shifting the apparent timing of climate transitions (Bard et al., 1987; Hutson, 1997). Currently, a constant concentration of the signal carrier is an assumption of *sedproxy*. Future work will enable climate dependent shifts in habitat and abundance to be modelled by implementing a parametrized response of proxy abundance and export to climate variables (Mix, 1987; Schmidt and Mulitza, 2002; Kretschmer et al., 2017; Jonkers and Kučera, 2017; Roche et al., 2017). An alternative option is to couple *sedproxy* to the output of ecological models that explicitly resolve the population dynamics of the proxy carrier, such as foraminifera population models (Fraile et al., 2008; Lombard et al., 2011).

For simplicity, we implemented a minimal physical model for bioturbation that assumes a completely mixed bioturbated layer, with a sharp cut-off to zero mixing below this layer (Berger and Heath, 1968). However, the general effect of bioturbation should also apply under conditions of incomplete mixing and the code could easily be modified to use a more complex bioturbation model (e.g., Guinasso and Schink, 1975; Steiner et al., 2016) to generate the weights used to sample the input climate signal. We note that when sedimentation rates are low relative to mixing rates, more complex mixing models converge to the simple box type model that we employ here (Matisoff, 1982).

Our model further assumes a constant bioturbation depth over time, as the bioturbation depth is generally not known for each setting and cannot easily be reconstructed down-core. Bioturbation depth may be related to productivity and sedimentation rate, but its predictability for a given core seems to be low (Trauth et al., 1997). The recent development of radiocarbon measurements on small samples (Wacker et al., 2010) might allow the extent of bioturbation to be constrained using replicate measurements from individual depth layers and such information could easily be included in *sedproxy*.

In contrast to some other proxy system models that have been proposed for corals, ice, trees and speleothems (e.g., Dee et al., 2015), *sedproxy* currently does not explicitly include the depth to age conversion and thus does not account for chronological uncertainty. In future studies, radiocarbon could be included in the forward modelling and thus the link between finite sample size, bioturbation and chronological uncertainty could be included.

Finally, in our examples we assumed that the climate signal recorded is that of the water column directly above the core location. There is evidence that this is not always the case, especially in dynamic regions and at drift deposits (Mollenhauer et al., 2003; van der Meer et al., 2017). This effect could be included by providing the non-local climate information as input to the forward model.

While *sedproxy* largely relies on well understood processes that have been previously described in the literature, there is a strong need to refine this and other proxy system models and to confront them with observational data. For this purpose, more systematic multiproxy studies comparing independent proxies from the same archives (e.g., Ho and Laepple, 2016; Laepple and Huybers, 2013; Weldeab et al., 2007; Cisneros et al., 2016) would be useful. Studies analysing replicability inside and between sediment cores in analogue to studies for ice and coral based proxies (DeLong et al., 2013; Smith et al., 2006;

Münch et al., 2016) would allow better constraint of the sample error parameter. Likewise, further investigation of potentially important processes occurring during the preservation of archived proxy signals (e.g., Münch et al., 2017; Zonneveld et al., 2007; Kim et al., 2009) would allow these to be included in proxy system models. Finally, modern core-top studies of individual foraminifera distributions (e.g., Haarmann et al., 2011) would allow further testing of the assumption that there is a direct link
5 between proxy variability and climate variability.

We hope that this tool will be useful to the paleoclimate research community and we hope that it can provide a starting point for a more complete future proxy system model for sediment proxies. We invite external contributions via the Bitbucket repository, <https://bitbucket.org/ecus/sedproxy>.

Code and data availability. The forward model *sedproxy* is implemented as an R package and its source code is available from the public git repository at <https://bitbucket.org/ecus/sedproxy>. The R package also contains the data needed for the examples. R code to run all the examples in this manuscript is contained in supplement S1. Source code for the specific *sedproxy* version used to create the examples in this manuscript is contained in supplement S2. An interactive example showing the main features of *sedproxy* can be accessed at <https://limnolrgy.shinyapps.io/sedproxy-shiny/>
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Competing interests. The authors declare that they have no conflict of interest.

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References

- Anand, P., Elderfield, H., and Conte, M. H.: Calibration of Mg/Ca Thermometry in Planktonic Foraminifera from a Sediment Trap Time Series, *Paleoceanography*, 18, 1050, <https://doi.org/10.1029/2002PA000846>, 2003.
- Anderson, D. M.: Attenuation of Millennial-Scale Events by Bioturbation in Marine Sediments, *Paleoceanography*, 16, 352–357, 2001.
- 5 Bard, E., Arnold, M., Duprat, J., Moyes, J., and Duplessy, J. C.: Reconstruction of the Last Deglaciation: Deconvolved Records of $\delta^{18}\text{O}$ Profiles, Micropaleontological Variations and Accelerator Mass Spectrometric ^{14}C Dating, *Climate Dynamics*, 1, 101–112, 1987.
- Barker, S., Greaves, M., and Elderfield, H.: A Study of Cleaning Procedures Used for Foraminiferal Mg/Ca Paleothermometry, *Geochemistry, Geophysics, Geosystems*, 4, 8407, <https://doi.org/10.1029/2003GC000559>, 2003.
- Barker, S., Cacho, I., Benway, H., and Tachikawa, K.: Planktonic Foraminiferal Mg/Ca as a Proxy for Past Oceanic Temperatures:
10 A Methodological Overview and Data Compilation for the Last Glacial Maximum, *Quaternary Science Reviews*, 24, 821–834, <https://doi.org/10.1016/j.quascirev.2004.07.016>, 2005.
- Barker, S., Broecker, W., Clark, E., and Hajdas, I.: Radiocarbon Age Offsets of Foraminifera Resulting from Differential Dissolution and Fragmentation within the Sedimentary Bioturbated Zone, *Paleoceanography*, 22, PA2205, <https://doi.org/10.1029/2006PA001354>, 2007.
- Benthien, A. and Müller, P. J.: Anomously Low Alkenone Temperatures Caused by Lateral Particle and Sediment Transport in the
15 Malvinas Current Region, Western Argentine Basin, *Deep Sea Research Part I: Oceanographic Research Papers*, 47, 2369–2393, [https://doi.org/10.1016/S0967-0637\(00\)00030-3](https://doi.org/10.1016/S0967-0637(00)00030-3), 2000.
- Berger, W. H. and Heath, G. R.: Vertical Mixing in Pelagic Sediments, *Journal of Marine Research*, 26, 134–143, 1968.
- Bijma, J., Erez, J., and Hemleben, C.: Lunar and Semi-Lunar Reproductive Cycles in Some Spinose Planktonic Foraminifers, *Journal of foraminiferal research*, 20, 117–127, 1990.
- 20 Black, D. E., Abahazi, M. A., Thunell, R. C., Kaplan, A., Tappa, E. J., and Peterson, L. C.: An 8-Century Tropical Atlantic SST Record from the Cariaco Basin: Baseline Variability, Twentieth-Century Warming, and Atlantic Hurricane Frequency, *Paleoceanography*, 22, PA4204, <https://doi.org/10.1029/2007PA001427>, 2007.
- Boudreau, B. P.: Mean Mixed Depth of Sediments: The Wherefore and the Why, *Limnology and Oceanography*, 43, 524–526, 1998.
- Cisneros, M., Cacho, I., Frigola, J., Canals, M., Masqué, P., Martrat, B., Casado, M., Grimalt, J. O., Pena, L. D., Margaritelli, G., and
25 Lirer, F.: Sea Surface Temperature Variability in the Central-Western Mediterranean Sea during the Last 2700 Years: A Multi-Proxy and Multi-Record Approach, *Climate of the Past*, 12, 849–869, <https://doi.org/10.5194/cp-12-849-2016>, 2016.
- Conte, M. H., Thompson, A., Lesley, D., and Harris, R. P.: Genetic and Physiological Influences on the Alkenone/Alkenoate versus Growth Temperature Relationship in *Emiliania Huxleyi* and *Gephyrocapsa Oceanica*, *Geochimica et Cosmochimica Acta*, 62, 51–68, 1998.
- Conte, M. H., Sicre, M.-A., Rühlemann, C., Weber, J. C., Schulte, S., Schulz-Bull, D., and Blanz, T.: Global Temperature Calibration
30 of the Alkenone Unsaturation Index (UK'37) in Surface Waters and Comparison with Surface Sediments, *Geochemistry Geophysics Geosystems*, 7, Q02 005, <https://doi.org/10.1029/2005GC001054>, 2006.
- Dee, S., Emile-Geay, J., Evans, M. N., Allam, A., Steig, E. J., and Thompson, D.: PRYSM: An Open-Source Framework for PROXY System Modeling, with Applications to Oxygen-Isotope Systems, *Journal of Advances in Modeling Earth Systems*, 7, 1220–1247, <https://doi.org/10.1002/2015MS000447>, 2015.
- 35 DeLong, K. L., Quinn, T. M., Taylor, F. W., Shen, C.-C., and Lin, K.: Improving Coral-Base Paleoclimate Reconstructions by Replicating 350 Years of Coral Sr/Ca Variations, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 373, 6–24, <https://doi.org/10.1016/j.palaeo.2012.08.019>, 2013.

- Douglass, A. E.: Climatic Cycles and Tree-Growth, Carnegie Institution of Washington, Washington, 1919.
- Dueñas-Bohórquez, A., da Rocha, R. E., Kuroyanagi, A., de Nooijer, L. J., Bijma, J., and Reichart, G.-J.: Interindividual Variability and Ontogenetic Effects on Mg and Sr Incorporation in the Planktonic Foraminifer *Globigerinoides Sacculifer*, *Geochimica et Cosmochimica Acta*, 75, 520–532, <https://doi.org/10.1016/j.gca.2010.10.006>, 2011.
- 5 Duplessy, J. C., Lalou, C., and Vinot, A. C.: Differential Isotopic Fractionation in Benthic Foraminifera and Paleotemperatures Reassessed, *Science*, 168, 250–251, <https://doi.org/10.1126/science.168.3928.250>, 1970.
- Elderfield, H. and Ganssen, G.: Past Temperature and $\Delta^{18}\text{O}$ of Surface Ocean Waters Inferred from Foraminiferal Mg/Ca Ratios, *Nature*, 405, 442–445, <https://doi.org/10.1038/35013033>, 2000.
- Evans, M. N., Tolwinski-Ward, S. E., Thompson, D. M., and Anchukaitis, K. J.: Applications of Proxy System Modeling in High Resolution Paleoclimatology, *Quaternary Science Reviews*, 76, 16–28, <https://doi.org/10.1016/j.quascirev.2013.05.024>, 2013.
- 10 Fairbanks, R. G. and Wiebe, P. H.: Foraminifera and Chlorophyll Maximum: Vertical Distribution, Seasonal Succession, and Paleoceanographic Significance, *Science*, 209, 1524–1526, <https://doi.org/10.1126/science.209.4464.1524>, 1980.
- Fraass, A. J. and Lowery, C. M.: Defining Uncertainty and Error in Planktic Foraminiferal Oxygen Isotope Measurements, *Paleoceanography*, 32, 2016PA003 035, <https://doi.org/10.1002/2016PA003035>, 2017.
- 15 Fraile, I., Schulz, M., Mulitza, S., and Kucera, M.: Predicting the Global Distribution of Planktonic Foraminifera Using a Dynamic Ecosystem Model, *Biogeosciences*, 5, 891–911, 2008.
- Fraile, I., Mulitza, S., and Schulz, M.: Modeling Planktonic Foraminiferal Seasonality: Implications for Sea-Surface Temperature Reconstructions, *Marine Micropaleontology*, 72, 1–9, <https://doi.org/10.1016/j.marmicro.2009.01.003>, 2009.
- Ganssen, G. M., Peeters, F. J. C., Metcalfe, B., Anand, P., Jung, S. J. A., Kroon, D., and Brummer, G.-J. A.: Quantifying Sea Surface Temperature Ranges of the Arabian Sea for the Past 20 000 Years, *Climate of the Past*, 7, 1337–1349, <https://doi.org/10.5194/cp-7-1337-2011>, 2011.
- 20 Goreau, T. J.: Frequency Sensitivity of the Deep-Sea Climatic Record, *Nature*, 287, 620, <https://doi.org/10.1038/287620a0>, 1980.
- Greaves, M., Caillon, N., Rebaubier, H., Bartoli, G., Bohaty, S., Cacho, I., Clarke, L., Cooper, M., Daunt, C., Delaney, M., deMenocal, P., Dutton, A., Eggins, S., Elderfield, H., Garbe-Schoenberg, D., Goddard, E., Green, D., Groeneveld, J., Hastings, D., Hathorne, E., Kimoto, K., Klinkhammer, G., Labeyrie, L., Lea, D. W., Marchitto, T., Martínez-Botí, M. A., Mortyn, P. G., Ni, Y., Nuernberg, D., Paradis, G., Pena, L., Quinn, T., Rosenthal, Y., Russell, A., Sagawa, T., Sosdian, S., Stott, L., Tachikawa, K., Tappa, E., Thunell, R., and Wilson, P. A.: Interlaboratory Comparison Study of Calibration Standards for Foraminiferal Mg/Ca Thermometry, *Geochemistry Geophysics Geosystems*, 9, 27 PP., [https://doi.org/2008%002010.1029/2008GC001974%0020\[Citation\]](https://doi.org/2008%002010.1029/2008GC001974%0020[Citation]), 2008.
- 25 Groeneveld, J., Hathorne, E., Steinke, S., DeBey, H., Mackensen, A., and Tiedemann, R.: Glacial Induced Closure of the Panamanian Gateway during Marine Isotope Stages (MIS) 95–100 (~2.5 Ma), *Earth and Planetary Science Letters*, 404, 296–306, <https://doi.org/10.1016/j.epsl.2014.08.007>, 2014.
- 30 Guinasso, N. L. G. and Schink, D. R.: Quantitative Estimates of Biological Mixing Rates in Abyssal Sediments, *Journal of Geophysical Research*, 80, PP. 3032–3043, <https://doi.org/10.1029/JC080i021p03032>, 1975.
- Haarmann, T., Hathorne, E. C., Mohtadi, M., Groeneveld, J., Kölling, M., and Bickert, T.: Mg/Ca Ratios of Single Planktonic Foraminifer Shells and the Potential to Reconstruct the Thermal Seasonality of the Water Column, *Paleoceanography*, 26, PA3218, <https://doi.org/10.1029/2010PA002091>, 2011.
- 35 Ho, S. L. and Laepple, T.: Flat Meridional Temperature Gradient in the Early Eocene in the Subsurface Rather than Surface Ocean, *Nature Geoscience*, 9, 606–610, <https://doi.org/10.1038/ngeo2763>, 2016.

- Hoefs, M. J. L., Versteegh, G. J. M., Rijpstra, W. I. C., de Leeuw, J. W., and Damsté, J. S. S.: Postdepositional Oxidic Degradation of Alkenones: Implications for the Measurement of Palaeo Sea Surface Temperatures, *Paleoceanography*, 13, PP. 42–49, <https://doi.org/199810.1029/97PA02893>, 1998.
- Hönisch, B., Allen, K. A., Lea, D. W., Spero, H. J., Eggins, S. M., Arbuszewski, J., deMenocal, P., Rosenthal, Y., Russell, A. D., and Elderfield, H.: The Influence of Salinity on Mg/Ca in Planktic Foraminifers – Evidence from Cultures, Core-Top Sediments and Complementary $\delta^{18}\text{O}$, *Geochimica et Cosmochimica Acta*, 121, 196–213, <https://doi.org/10.1016/j.gca.2013.07.028>, 2013.
- Hutson, W. H.: Bioturbation of Deep-Sea Sediments: Oxygen Isotopes and Stratigraphic Uncertainty, *Geology*, 8, 127–130, [https://doi.org/10.1130/0091-7613\(1980\)8<127:BODSOI>2.0.CO;2](https://doi.org/10.1130/0091-7613(1980)8<127:BODSOI>2.0.CO;2), 1980.
- Jonkers, L. and Kučera, M.: Global Analysis of Seasonality in the Shell Flux of Extant Planktonic Foraminifera, *Biogeosciences*, 12, 2207–2226, <https://doi.org/10.5194/bg-12-2207-2015>, 2015.
- Jonkers, L. and Kučera, M.: Quantifying the Effect of Seasonal and Vertical Habitat Tracking on Planktonic Foraminifera Proxies, *Climate of the Past*, 13, 573–586, <https://doi.org/10.5194/cp-13-573-2017>, 2017.
- Killingley, J. S., Johnson, R. F., and Berger, W. H.: Oxygen and Carbon Isotopes of Individual Shells of Planktonic Foraminifera from Ontong-Java Plateau, Equatorial Pacific, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 33, 193–204, [https://doi.org/10.1016/0031-0182\(81\)90038-9](https://doi.org/10.1016/0031-0182(81)90038-9), 1981.
- Kim, J.-H., Huguet, C., Zonneveld, K. A., Versteegh, G. J., Roeder, W., Sinninghe Damsté, J. S., and Schouten, S.: An Experimental Field Study to Test the Stability of Lipids Used for the TEX86 and Palaeothermometers, *Geochimica et Cosmochimica Acta*, 73, 2888–2898, <https://doi.org/10.1016/j.gca.2009.02.030>, 2009.
- Klein, F. and Goussé, H.: Reconstructing East African Rainfall and Indian Ocean Sea Surface Temperatures over the Last Centuries Using Data Assimilation, *Climate Dynamics*, pp. 1–21, <https://doi.org/10.1007/s00382-017-3853-0>, 2017.
- Koutavas, A. and Joannides, S.: El Niño–Southern Oscillation Extrema in the Holocene and Last Glacial Maximum, *Paleoceanography*, 27, PA4208, <https://doi.org/10.1029/2012PA002378>, 2012.
- Kretschmer, K., Jonkers, L., Kucera, M., and Schulz, M.: Modeling Seasonal and Vertical Habitats of Planktonic Foraminifera on a Global Scale, *Biogeosciences Discussions*, pp. 1–37, <https://doi.org/10.5194/bg-2017-429>, 2017.
- Laepple, T. and Huybers, P.: Reconciling Discrepancies between $\text{Uk}37$ and Mg/Ca Reconstructions of Holocene Marine Temperature Variability, *Earth and Planetary Science Letters*, 375, 418–429, <https://doi.org/10.1016/j.epsl.2013.06.006>, 2013.
- Laepple, T. and Huybers, P.: Ocean Surface Temperature Variability: Large Model–Data Differences at Decadal and Longer Periods, *Proceedings of the National Academy of Sciences*, 111, 16 682–16 687, <https://doi.org/10.1073/pnas.1412077111>, 2014.
- Leduc, G., Schneider, R., Kim, J., and Lohmann, G.: Holocene and Eemian Sea Surface Temperature Trends as Revealed by Alkenone and Mg/Ca Paleothermometry, *Quaternary science reviews*, 29, 989–1004, 2010.
- Liu, Z., Otto-Bliesner, B. L., He, F., Brady, E. C., Tomas, R., Clark, P. U., Carlson, A. E., Lynch-Stieglitz, J., Curry, W., Brook, E., Erickson, D., Jacob, R., Kutzbach, J., and Cheng, J.: Transient Simulation of Last Deglaciation with a New Mechanism for Bølling–Allerød Warming, *Science*, 325, 310–314, <https://doi.org/10.1126/science.1171041>, 2009.
- Liu, Z., Zhu, J., Rosenthal, Y., Zhang, X., Otto-Bliesner, B. L., Timmermann, A., Smith, R. S., Lohmann, G., Zheng, W., and Timm, O. E.: The Holocene Temperature Conundrum, *Proceedings of the National Academy of Sciences*, 111, E3501–E3505, <https://doi.org/10.1073/pnas.1407229111>, 2014.
- Lohmann, G., Pfeiffer, M., Laepple, T., Leduc, G., and Kim, J.-H.: A Model–Data Comparison of the Holocene Global Sea Surface Temperature Evolution, *Clim. Past*, 9, 1807–1839, <https://doi.org/10.5194/cp-9-1807-2013>, 2013.

- Lombard, F., Labeyrie, L., Michel, E., Bopp, L., Cortijo, E., Retailleau, S., Howa, H., and Jorissen, F.: Modelling Planktic Foraminifer Growth and Distribution Using an Ecophysiological Multi-Species Approach, *Biogeosciences*, 8, 853–873, <https://doi.org/10.5194/bg-8-853-2011>, 2011.
- Lougheed, B. C., Metcalfe, B., Ninnemann, U. S., and Wacker, L.: Moving beyond the Age-Depth Model Paradigm in Deep Sea Palaeoclimate Archives: Dual Radiocarbon and Stable Isotope Analysis on Single Foraminifera, *Clim. Past Discuss.*, 2017, 1–16, <https://doi.org/10.5194/cp-2017-119>, 2017.
- Matisoff, G.: Mathematical Models of Bioturbation, in: *Animal-Sediment Relations: The Biogenic Alteration of Sediments*, edited by McCall, P. L. and Tevesz, M. J. S., pp. 289–330, Springer, New York, 1982.
- Mekik, F., François, R., and Soon, M.: A Novel Approach to Dissolution Correction of Mg/Ca–Based Paleothermometry in the Tropical Pacific, *Paleoceanography*, 22, n/a–n/a, <https://doi.org/10.1029/2007PA001504>, 2007.
- Mix, A.: The Oxygen-Isotope Record of Glaciation, in: *North America and Adjacent Oceans during the Last Deglaciation.*, vol. K-3 of *Geology of North America*, pp. 111–135, Geological Society of America, 1987.
- Mollenhauer, G., Eglinton, T. I., Ohkouchi, N., Schneider, R. R., Müller, P. J., Grootes, P. M., and Rullkötter, J.: Asynchronous Alkenone and Foraminifera Records from the Benguela Upwelling System, *Geochimica et Cosmochimica Acta*, 67, 2157–2171, [https://doi.org/10.1016/S0016-7037\(03\)00168-6](https://doi.org/10.1016/S0016-7037(03)00168-6), 2003.
- Müller, P. J., Kirst, G., Ruhland, G., von Storch, I., and Rosell-Melé, A.: Calibration of the Alkenone Paleotemperature Index U37K' Based on Core-Tops from the Eastern South Atlantic and the Global Ocean (60 N-60 S), *Geochimica et Cosmochimica Acta*, 62, 1757–1772, [https://doi.org/10.1016/S0016-7037\(98\)00097-0](https://doi.org/10.1016/S0016-7037(98)00097-0), 1998.
- Münch, T., Kipfstuhl, S., Freitag, J., Meyer, H., and Laepple, T.: Regional Climate Signal vs. Local Noise: A Two-Dimensional View of Water Isotopes in Antarctic Firn at Kohlen Station, Dronning Maud Land, *Clim. Past*, 12, 1565–1581, <https://doi.org/10.5194/cp-12-1565-2016>, 2016.
- Münch, T., Kipfstuhl, S., Freitag, J., Meyer, H., and Laepple, T.: Constraints on Post-Depositional Isotope Modifications in East Antarctic Firn from Analysing Temporal Changes of Isotope Profiles, *The Cryosphere*, 11, 2175–2188, <https://doi.org/10.5194/tc-11-2175-2017>, 2017.
- Nürnberg, D., Bijma, J., and Hemleben, C.: Assessing the Reliability of Magnesium in Foraminiferal Calcite as a Proxy for Water Mass Temperatures, *Geochimica et Cosmochimica Acta*, 60, 803–814, [https://doi.org/10.1016/0016-7037\(95\)00446-7](https://doi.org/10.1016/0016-7037(95)00446-7), 1996.
- Prahl, F. G. and Wakeham, S. G.: Calibration of Unsaturation Patterns in Long-Chain Ketone Compositions for Palaeotemperature Assessment, *Nature*, 330, 367, <https://doi.org/10.1038/330367a0>, 1987.
- R Core Team: R: A Language and Environment for Statistical Computing, Vienna, Austria, 2017.
- Roche, D. M., Waelbroeck, C., Metcalfe, B., and Caley, T.: FAME (v1.0): A Simple Module to Simulate the Effect of Planktonic Foraminifer Species-Specific Habitat on Their Oxygen Isotopic Content, *Geosci. Model Dev. Discuss.*, 2017, 1–22, <https://doi.org/10.5194/gmd-2017-251>, 2017.
- Rosell-Melé, A., Bard, E., Emeis, K.-C., Grimalt, J. O., Müller, P., Schneider, R., Bouloubassi, I., Epstein, B., Fahl, K., Fluegge, A., Freeman, K., Goñi, M., Güntner, U., Hartz, D., Hellebust, S., Herbert, T., Ikehara, M., Ishiwatari, R., Kawamura, K., Kenig, F., de Leeuw, J., Lehman, S., Mejanelle, L., Ohkouchi, N., Pancost, R. D., Pelejero, C., Prahl, F., Quinn, J., Rontani, J.-F., Rostek, F., Rullkötter, J., Sachs, J., Blanz, T., Sawada, K., Schulz-Bull, D., Sikes, E., Sonzogni, C., Ternois, Y., Versteegh, G., Volkman, J., and Wakeham, S.: Precision of the Current Methods to Measure the Alkenone Proxy UK'37 and Absolute Alkenone Abundance in Sediments: Results of an Interlaboratory Comparison Study, *Geochemistry Geophysics Geosystems*, 2, Paper number 2000GC0, 2001.

- Rosenthal, Y. and Lohmann, G. P.: Accurate Estimation of Sea Surface Temperatures Using Dissolution-Corrected Calibrations for Mg/Ca Paleothermometry, *Paleoceanography*, 17, 1044, <https://doi.org/10.1029/2001PA000749>, 2002.
- Rosenthal, Y., Oppo, D. W., and Linsley, B. K.: The Amplitude and Phasing of Climate Change during the Last Deglaciation in the Sulu Sea, Western Equatorial Pacific, *Geophysical Research Letters*, 30, 1428, <https://doi.org/10.1029/2002GL016612>, 2003.
- 5 Sadekov, A., Eggins, S. M., De Deckker, P., and Kroon, D.: Uncertainties in Seawater Thermometry Deriving from Intratest and Interest Mg/Ca Variability in *Globigerinoides Ruber*: UNCERTAINTIES Mg/Ca SEAWATER THERMOMETRY, *Paleoceanography*, 23, n/a–n/a, <https://doi.org/10.1029/2007PA001452>, 2008.
- Sadler, P. M.: The Influence of Hiatuses on Sediment Accumulation Rates, in: *GeoResearch Forum*, vol. 5, 1999.
- Schiffelbein, P. and Hills, S.: Direct Assessment of Stable Isotope Variability in Planktonic Foraminifera Populations, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 48, 197–213, [https://doi.org/10.1016/0031-0182\(84\)90044-0](https://doi.org/10.1016/0031-0182(84)90044-0), 1984.
- 10 Schmidt, G. A. and Mulitza, S.: Global Calibration of Ecological Models for Planktic Foraminifera from Coretop Carbonate Oxygen-18, *Marine Micropaleontology*, 44, 125–140, [https://doi.org/10.1016/S0377-8398\(01\)00041-X](https://doi.org/10.1016/S0377-8398(01)00041-X), 2002.
- Schneider, B., Leduc, G., and Park, W.: Disentangling Seasonal Signals in Holocene Climate Trends by Satellite-Model-Proxy Integration, *Paleoceanography*, 25, PA4217, <https://doi.org/10.1029/2009PA001893>, 2010.
- 15 Scussolini, P. and Peeters, F. J. C.: A Record of the Last 460 Thousand Years of Upper Ocean Stratification from the Central Walvis Ridge, South Atlantic, *Paleoceanography*, 28, 426–439, <https://doi.org/10.1002/palo.20041>, 2013.
- Scussolini, P., van Sebille, E., and Durgadoo, J. V.: Paleo Agulhas Rings Enter the Subtropical Gyre during the Penultimate Deglaciation, *Climate of the Past*, 9, 2631–2639, <https://doi.org/10.5194/cp-9-2631-2013>, 2013.
- Scussolini, P., Marino, G., Brummer, G.-J. A., and Peeters, F. J. C.: Saline Indian Ocean Waters Invaded the South Atlantic Thermocline during Glacial Termination II, *Geology*, 43, 139–142, <https://doi.org/10.1130/G36238.1>, 2015.
- 20 Shakun, J. D., Clark, P. U., He, F., Marcott, S. A., Mix, A. C., Liu, Z., Otto-Bliesner, B., Schmittner, A., and Bard, E.: Global Warming Preceded by Increasing Carbon Dioxide Concentrations during the Last Deglaciation, *Nature*, 484, 49–54, <https://doi.org/10.1038/nature10915>, 2012.
- Skinner, L. C. and Elderfield, H.: Constraining Ecological and Biological Bias in Planktonic Foraminiferal Mg/Ca and $\delta^{18}\text{O}_{\text{cc}}$: A Multi-species Approach to Proxy Calibration Testing, *Paleoceanography*, 20, PA1015, <https://doi.org/10.1029/2004PA001058>, 2005.
- Smerdon, J. E., Kaplan, A., Zorita, E., González-Rouco, J. F., and Evans, M. N.: Spatial Performance of Four Climate Field Reconstruction Methods Targeting the Common Era, *Geophysical Research Letters*, 38, L11 705, <https://doi.org/10.1029/2011GL047372>, 2011.
- Smith, J., Quinn, T., Helmle, K., and Halley, R.: Reproducibility of Geochemical and Climatic Signals in the Atlantic Coral *Montastraea Faveolata*, *Paleoceanography*, 21, 2006.
- 30 Sommerfield, C. K.: On Sediment Accumulation Rates and Stratigraphic Completeness: Lessons from Holocene Ocean Margins, *Continental Shelf Research*, 26, 2225–2240, <https://doi.org/10.1016/j.csr.2006.07.015>, 2006.
- Spero, H. J.: Life History and Stable Isotope Geochemistry of Planktonic Foraminifera, *The Paleontological Society Papers*, 4, 7–36, <https://doi.org/10.1017/S1089332600000383>, 1998.
- Steiner, Z., Lazar, B., Levi, S., Tsroya, S., Pelled, O., Bookman, R., and Erez, J.: The Effect of Bioturbation in Pelagic Sediments: Lessons from Radioactive Tracers and Planktonic Foraminifera in the Gulf of Aqaba, Red Sea, *Geochimica et Cosmochimica Acta*, 194, 139–152, <https://doi.org/10.1016/j.gca.2016.08.037>, 2016.
- 35 Teal, L., Bulling, M., Parker, E., and Solan, M.: Global Patterns of Bioturbation Intensity and Mixed Depth of Marine Soft Sediments, *Aquatic Biology*, 2, 207–218, <https://doi.org/10.3354/ab00052>, 2010.

- Thirumalai, K., Partin, J. W., Jackson, C. S., and Quinn, T. M.: Statistical Constraints on El Niño Southern Oscillation Reconstructions Using Individual Foraminifera: A Sensitivity Analysis, *Paleoceanography*, 28, 401–412, <https://doi.org/10.1002/palo.20037>, 2013.
- Tingley, M. P. and Huybers, P.: A Bayesian Algorithm for Reconstructing Climate Anomalies in Space and Time. Part I: Development and Applications to Paleoclimate Reconstruction Problems, *Journal of Climate*, 23, 2759–2781, <https://doi.org/10.1175/2009JCLI3015.1>,
5 2009.
- Trauth, M. H., Sarnthein, M., and Arnold, M.: Bioturbational Mixing Depth and Carbon Flux at the Seafloor, *Paleoceanography*, 12, 517–526, <https://doi.org/10.1029/97PA00722>, 1997.
- Uitz, J., Claustre, H., Gentili, B., and Stramski, D.: Phytoplankton Class-Specific Primary Production in the World’s Oceans: Seasonal and Interannual Variability from Satellite Observations, *Global Biogeochemical Cycles*, 24, n/a–n/a, <https://doi.org/10.1029/2009GB003680>,
10 2010.
- van Sebille, E., Scussolini, P., Durgadoo, J. V., Peeters, F. J. C., Biastoch, A., Weijer, W., Turney, C., Paris, C. B., and Zahn, R.: Ocean Currents Generate Large Footprints in Marine Palaeoclimate Proxies, *Nature Communications*, 6, 6521, <https://doi.org/10.1038/ncomms7521>, 2015.
- Wacker, L., Bonani, G., Friedrich, M., Hajdas, I., Kromer, B., Nemeč, N., Ruff, M., Suter, M., Synal, H.-A., and Vockenhuber, C.: MICADAS: Routine and High-Precision Radiocarbon Dating, *Radiocarbon*, 52, 252–262, 2010.
- Weldeab, S., Schneider, R. R., and Müller, P.: Comparison of Mg/Ca- and Alkenone-Based Sea Surface Temperature Estimates in the Fresh Water–Influenced Gulf of Guinea, Eastern Equatorial Atlantic, *Geochemistry, Geophysics, Geosystems*, 8, Q05P22, <https://doi.org/10.1029/2006GC001360>, 2007.
- Wickham, H.: *Ggplot2: Elegant Graphics for Data Analysis*, Springer-Verlag New York, 2009.
- 20 Wit, J. C., Reichart, G.-J., A Jung, S. J., and Kroon, D.: Approaches to Unravel Seasonality in Sea Surface Temperatures Using Paired Single-Specimen Foraminiferal $\delta^{18}\text{O}$ and Mg/Ca Analyses, *Paleoceanography*, 25, PA4220, <https://doi.org/10.1029/2009PA001857>, 2010.
- Wörmer, L., Elvert, M., Fuchser, J., Lipp, J. S., Buttigieg, P. L., Zabel, M., and Hinrichs, K.-U.: Ultra-High-Resolution Paleoenvironmental Records via Direct Laser-Based Analysis of Lipid Biomarkers in Sediment Core Samples, *Proceedings of the National Academy of Sciences*, 111, 15 669–15 674, <https://doi.org/10.1073/pnas.1405237111>, 2014.
- 25 Zachos, J., Pagani, M., Sloan, L., Thomas, E., and Billups, K.: Trends, Rhythms, and Aberrations in Global Climate 65 Ma to Present, *Science*, 292, 686–693, <https://doi.org/10.1126/science.1059412>, 2001.
- Zonneveld, K. A., Bockelmann, F., and Holzwarth, U.: Selective Preservation of Organic-Walled Dinoflagellate Cysts as a Tool to Quantify Past Net Primary Production and Bottom Water Oxygen Concentrations, *Marine Geology*, 237, 109–126, <https://doi.org/10.1016/j.margeo.2006.10.023>, 2007.

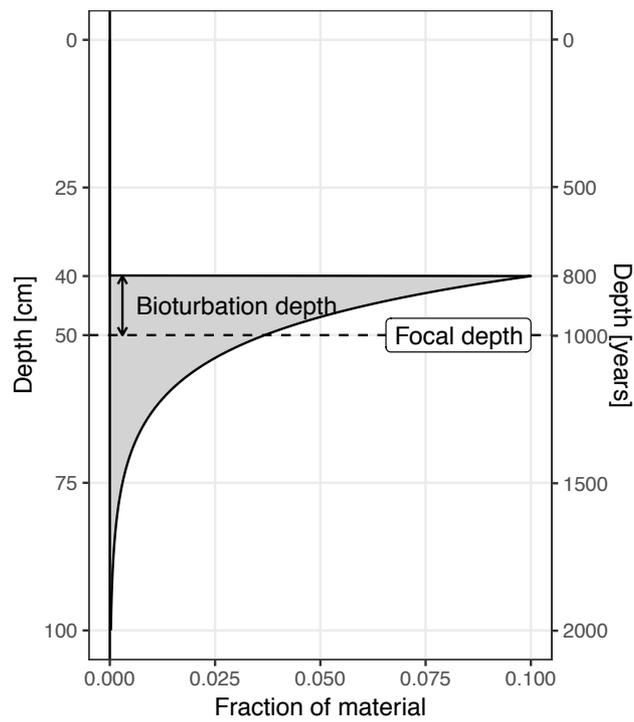


Figure 1. The origin of material archived at a focal core depth of 50 cm. In this example the bioturbation depth is 10 cm, and the sediment accumulation rate is 50 cm ka^{-1}

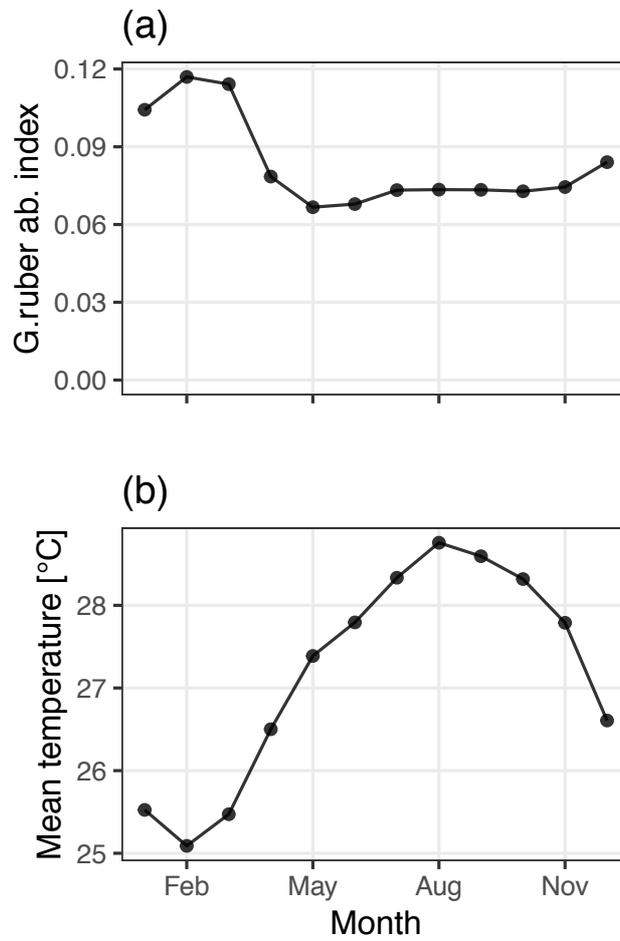


Figure 2. ~~Modelled abundance~~ Abundance index of *G.ruber* from PLAFOM (Fraile et al., 2008) (a), and the mean monthly sea surface temperature in the TraCE21ka simulation at MD97-2141 (b) at MD97-2141. In this model, *G.ruber* occurs over the whole year with a small maximum during the cooler months of Jan-March, therefore biasing the recorded temperature towards colder temperatures.

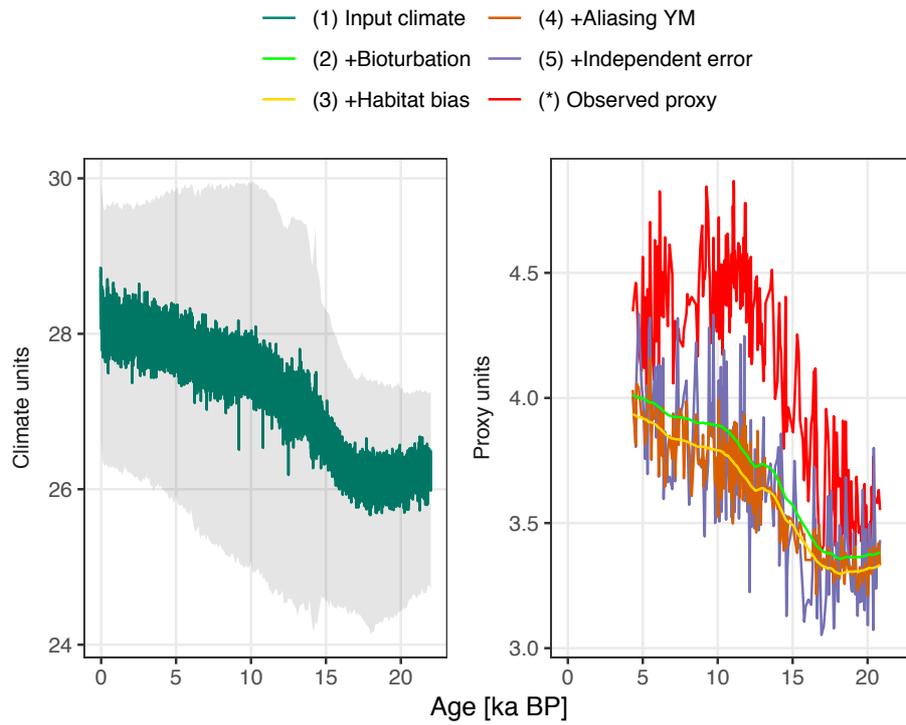


Figure 3. A forward modelled foraminiferal Mg/Ca pseudo-proxy record together with the observed Mg/Ca proxy record at core MD97-2141 in the Sulu Sea. The input climate is shown at annual resolution [with the full monthly input timeseries in grey](#).

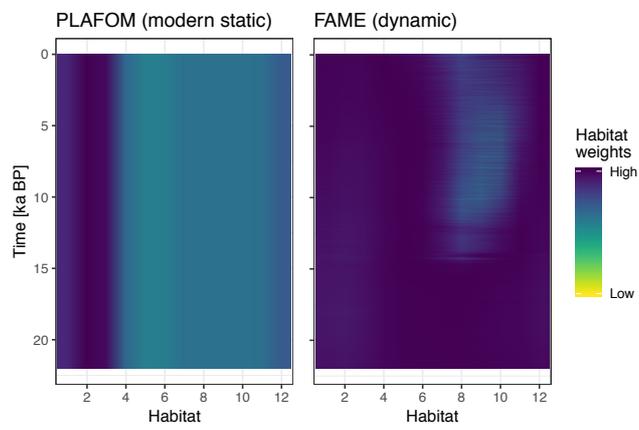


Figure 4. A comparison of static and dynamic monthly weights generated by PLAFOM driven by modern climatology, and FAME driven by the input climate matrix.

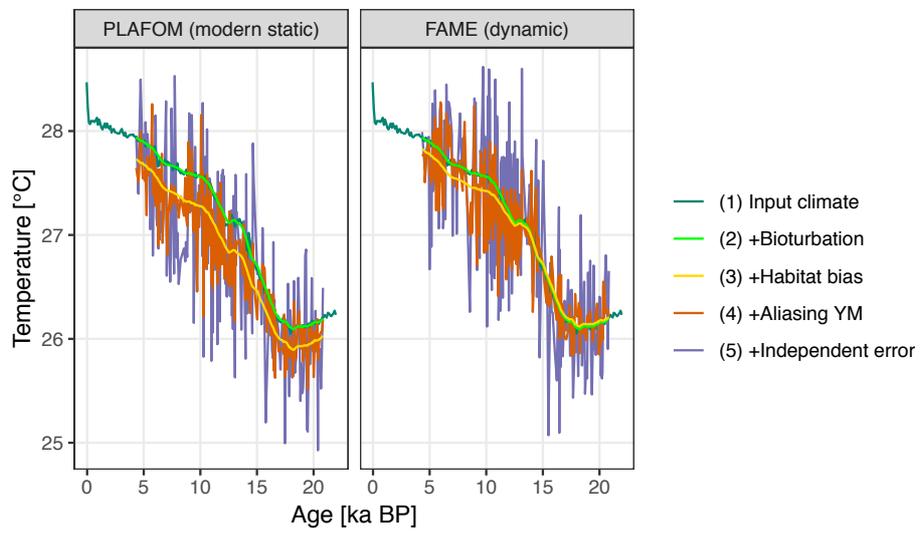


Figure 5. A comparison of forward modelled Mg/Ca based pseudo-proxies using static and dynamic seasonal weighting.

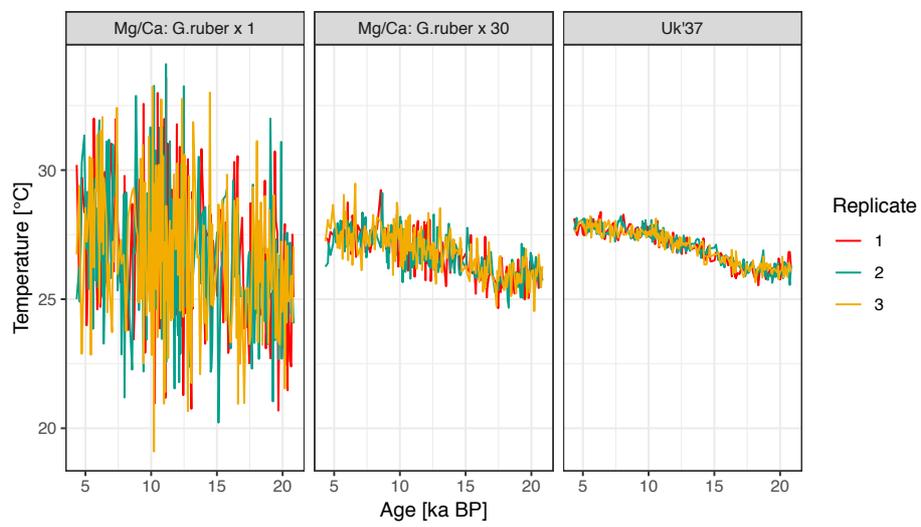


Figure 6. Forward modelled proxy based temperature reconstructions for Mg/Ca with 1 and 30 tests of *G.ruber*, and for Uk'37. [Three replicate runs of the forward model are shown.](#)

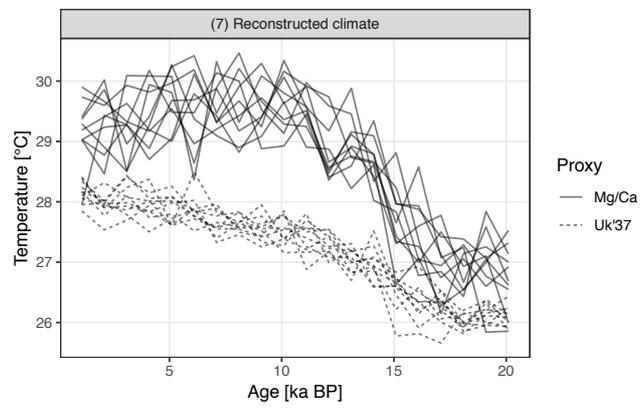
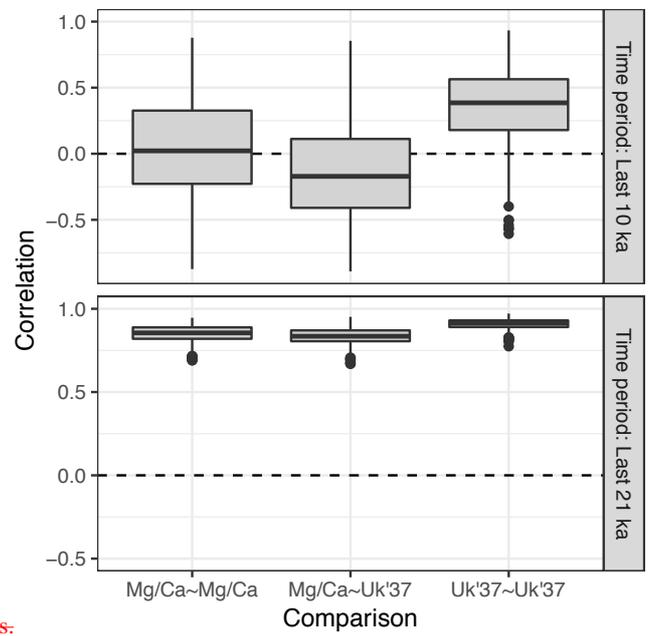


Figure 7. Replicate hypothetical Mg/Ca and Uk'37 based records. The two proxy types sample different parts of the seasonal cycle. Ten replicate records are shown for each proxy.



Correlation between replicate pairs of forward modelled proxy records:

Figure 8. [Correlation between replicate pairs of forward modelled proxy records.](#)

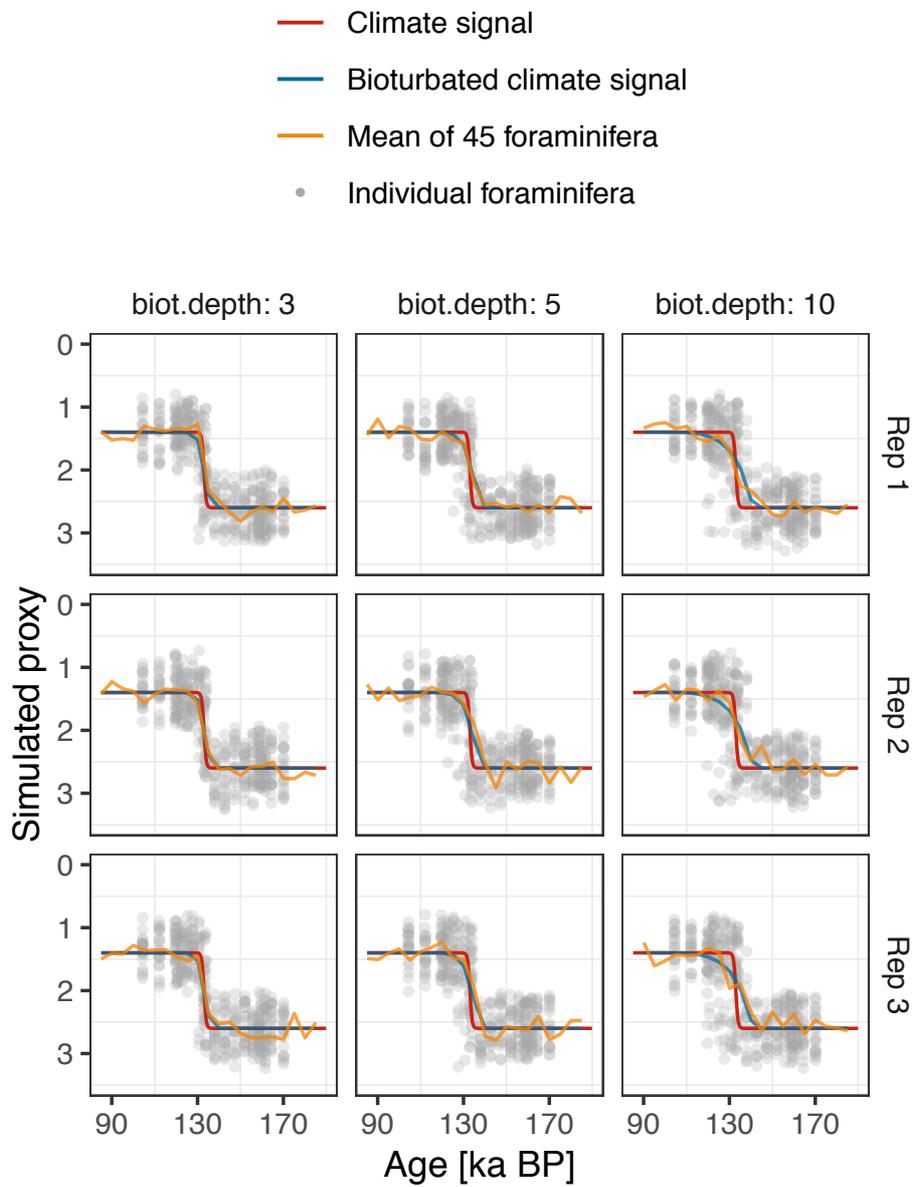


Figure 9. Simulated $\delta^{18}\text{O}$ measured from single foraminiferal tests (circles) and bulk samples (lines). Subplots show six replications with the same parameterisation.

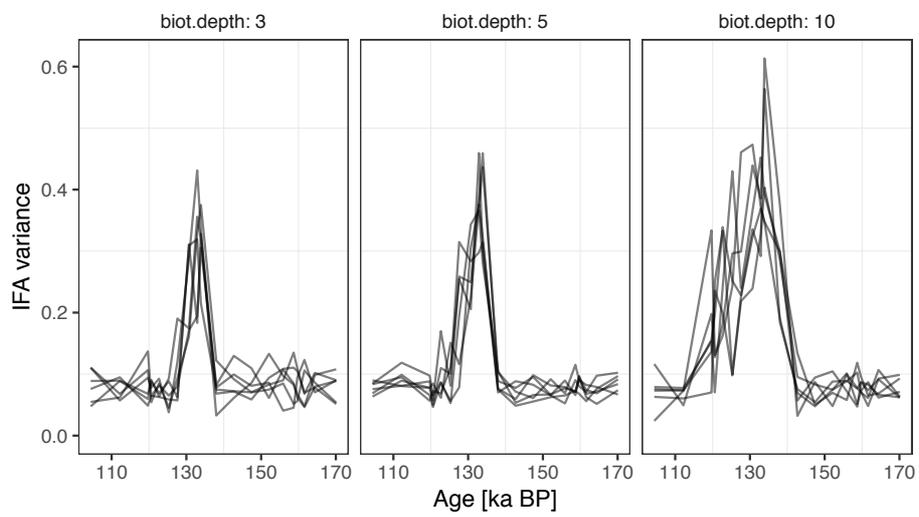


Figure 10. Variance in simulated $\delta^{18}\text{O}$ measured on sets of 20 individual foraminiferal tests. Lines show six replications with the same ~~parameterisation~~parametrisation.

Table 1. Required input data and parameters to generate a pseudo-proxy record with *sedproxy*. The final ~~two arguments control~~ argument controls the experimental design rather than the proxy record creation process itself.

Function argument

clim.signal

timepoints

~~proxy.prod.~~ calibration.type

Table 2. Details for sediment core MD97-2141

Core	Location	Lat	Lon	Proxy	Foram.sp	Reference
MD97-2141	Sulu Sea	8.78	121.28	Mg/Ca	G. ruber	Rosenthal et al., 2003