**Uneven spatial sampling in Phanerozoic palaeotemperature curves**

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# ABSTRACT

# INTRODUCTION

The geological record provides critical context for understanding past and current climate change (Alley et al., 2003). Measurements of the ratio of the stable isotopes oxygen-18 and oxygen-16 (δ18O) from the skeletons of fossil calcitic organisms enables reconstruction of palaeotemperatures. Today, δ18O measurements provide the most comprehensive palaeotemperature record of the Phanerozoic (Veizer and Prokoph, 2015; Grossman and Joachimski, 2020). The 18O/16O ratio of a pristine shell or skeleton is a function of the δ18O within the seawater during formation, and the temperature at the time of calcification (Urey, 1947; Horita and Wesolowski, 1994; Leng and Lewis, 2016). Typically, δ18O values are derived from shells or skeletons made of calcium carbonate, such as foraminifera, brachiopods, belemnites, bivalves and gastropods (Jones and Quitmyer, 1996), or from calcium phosphate, most notably from conodont skeletal elements (Wenzel et al., 2000). For the last 125 million years (myr), δ18O values are mostly derived from foraminifers, while brachiopod, conodont, belemnite and bivalve skeletons are the principal temperature archive of older formations (Veizer and Prokoph, 2015; Grossman and Joachimski, 2020).

Despite their wide application, several biases may impact δ18O measurements derived from fossil material. Diagenetic alteration is often considered the main bias, which alters the isotopic composition of the fossil material after its initial formation towards the isotopic composition of the pore water (Dickson and Coleman, 1980; Killingley, 1983; Schrag et al., 1995). Diagenetic effects (e.g. recrystallisation or the precipitation of additional calcite) have the potential to increase or decrease the calculated temperature by several degrees Celsius (Killingley, 1983). Careful screening of fossil material is required to retain only pristine material. However, even when using techniques such as cathodoluminescence or scanning electron microscopy (van Geldern et al., 2006), diagenetic alteration is not always easily identified. Fossil derived δ18O may also be impacted by ‘subsampling heterogeneities’, which may exist in a single sample, or within a sample constituted of several fossils. For example, the fossil shell can be segmented by sub-resolution growth bands containing different δ18O content (Klein et al., 1996; Jones and Quitmyer, 1996). In addition, growth bands can also be largest during the summer time, leading to higher measured temperatures than the global average ocean temperature (Mii and Grossman, 1994; Watanabe et al., 2001). ‘Vital effects’ are also considered an important bias in reconstructing past temperatures from fossil material. Vital effects refer to the observed offset between the in-situ temperature at which the shell is crystallized, and the temperature calculated from the carbonate shell (Epstein et al., 1951; Urey et al., 1951; Weiner and Dove, 2003). These vital effects are thought to be caused by kinetic effects during metabolic reactions, which drive δ18O away from the value predicted at equilibrium. However, vital effects have been widely studied and several experiments have helped to correct for this effect (Wefer and Berger, 1991).

Whilst the impact of the aforementioned biases is relatively well-known, a potential bias on estimates of global temperature has been largely overlooked—the spatial coverage of fossil samples, and their respective δ18O values. The spatial distribution and number of δ18O measurements has the potential to strongly influence global estimates of palaeotemperature. To provide an example, if the arithmetic mean of 100 δ18O derived palaeotemperatures is used to represent the global stage-level palaeotemperature, and 90 measurements are from tropical latitudes, this will likely overestimate the ‘global’ mean temperature. Equally, if the spatial distribution of our δ18O measurements shifts between time bins, observed changes in global temperature might be a result of the shift in spatial distribution of the δ18O measurements. Accordingly, we hypothesize that the heterogeneous spatial distribution of palaeotemperature proxy records impacts our understanding of the evolution of global temperature through geological time.

To test this hypothesis, we used an extensive Phanerozoic compilation of δ18O measurements from the Stable Isotope Database (StabisoDB), and quantified the spatiotemporal evolution of sampling. Building upon this analysis, we implemented a parsimonious approach in which we evaluated the difference between a global representative model of sea surface temperature (SST) today, and what the estimate of SST would be based on the spatial distribution of δ18O measurements.

# MATERIALS AND METHODS

## Dataset

Measurements of δ18O across the Phanerozoic (XXX–2.59 Ma) were downloaded from the StabisoDB (<https://cnidaria.nat.uni-erlangen.de/stabisodb/>) on the 2nd December 2020. This database provides an open-access dataset of stable isotope measurements, and builds upon previous published compilations (e.g. Veizer and Prokoph, 2015; Grossman and Joachimski, 2020). These previous compilations have been extensively used in a range of past studies, including palaeoclimatology (Mills et al., 2019; Song et al., 2019) and palaeobiology (e.g. Mannion et al., 2015; Zapalski et al., 2017; Eichenseer et al., 2019). A total of XXX δ18O measurements were yielded at the time of download, with XXX remaining after data cleaning. For the purposes of this study, we removed measurements that: (1) lacked geographic coordinates; (2) were not constrained to stratigraphic stage level; (3) lacked δ18O values; (4) were derived from problematic taxonomic groups; and (5) mineralogies other than ‘aragonite’ or ‘calcite’ (see SI for justification). In accordance with previous work, we calculated palaeotemperatures using the δ18O (‰ PDB) to *T* (℃) transfer function from Veizer at al (2015), including a Phanerozoic trend of increasing δ18O as in equation (2) of Veizer at al (2015), with *t* denoting the age in million years before present:

For this study, data were temporally binned at stratigraphic stage-level using XXX. To enable our spatial analyses, δ18O measurements were palaeorotated using GPlates (Müller et al., 2018) via the reconstruction() function in the R package ‘chronosphere’ ver. 0.4.0 (Kocsis and Raja, 2019). Each data point was palaeorotated to the mid-age of its respective temporal bin, on the basis of its present-day coordinates. For our palaeorotations, we opted to use the ‘PALEOMAP’ plate reconstruction model [(Scotese and Wright 2018)](https://www.zotero.org/google-docs/?s7tc55), which is the standard rotation model integrated within the Palaeobiology Database (<https://paleobiodb.org/>), a global database of fossil occurrences, and the basis for numerous palaeontological studies.

## Spatial sampling metrics

To quantify the spatiotemporal evolution of sampling, we calculated three metrics within each stratigraphic stage-level bin: (1) the absolute palaeolatitudinal centroid of δ18O data; (2) the number of occupied equal-area grid cells; and (3) the summed minimum-spanning tree (MST) length between the palaeogeographic points of δ18O measurements. Equal area-grid cells were generated using the R package ‘dggridR’ (Barnes et al., 2017), with 100 km spacings, resulting in cells with an area of ~8,000 km2. The number of occupied equal-area grid cells (i.e. cells containing at least one δ18O measurement) provides a measure of sampling coverage. The summed MST length between palaeogeographic points was calculated using the spantree() function from the R package ‘vegan’ (Oksanen et al., 2019), and provides a measure of the spatial extent of sampling. As both land and sea surface temperature broadly follow a latitudinal gradient, with coolest temperatures at the poles, temporal shifts in the palaeolatitudinal sampling window may influence estimates of palaeotemperature. The absolute palaeolatitudinal centroid provides insight into whether temporal shifts in palaeotemperature are driven by shifts in the spatial sampling window or are a genuine signal (e.g. apparent cooling driven by a poleward shift in sampling).

## Empirical comparisons

To evaluate the influence of the spatiotemporal distribution of δ18O measurements on estimates of global SST, we used the palaeocoordinates of our dataset to extract temperature values from a global grid of SST. As some δ18O values originate from epicontinental seaways (i.e. terrestrial environments today), extracting a direct value of present-day SST was not possible. Therefore, we generated a hypothetical SST grid by calculating the mean longitudinal SST across a latitudinal axis for a grid (spatial resolution of 5 arcmin) of present-day mean annual SST, downloaded from Bio-ORACLE (Tyberghein et al. 2012). Using the extracted SST values, we calculated the observed mean annual ‘global’ SST based on the spatial distribution of the data at stage-level, and compared the difference between the known ‘hypothetical’ global SST (XXX) and the observed global SST. All data analyses were performed in R ver. 4.0.3, and the code is available in the supplementary information.

# RESULTS

* Spatial distribution of data/with time
* Temperature curve
* Reef data/linear model

# DISCUSSION

* Issues with original data
* New improved model
* Empirical support for new curve
* Limitations and future directions

# CONCLUSION

# DATA ACCESSIBILITY

All supplementary material and data have been included as part of the submission. All analyses were performed in R ver. 4.0.3, and are available on GitHub (accessible via: XXX)

# AUTHOR’S CONTRIBUTIONS

LAJ and KE conceived and designed the project, developed and performed the analyses, and interpreted the data. All authors contributed to the writing of the manuscript. LAJ and KE produced the figures.

# COMPETING INTERESTS

We declare we have no competing interests.

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