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Robust multi-proxy data integration, using late Cretaceous paleotemperature records as a case study

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ABSTRACT

In paleoclimate studies, multiple temperature records are often compared and combined to evaluate temperature trends. Yet, no standardized approach for integrating proxy-derived paleotemperature records exists. In addition, paleotemperature data are often reported without uncertainty estimates (prediction errors), and raw data are not always available. This complicates the quantification of, for example, temperature trends and the magnitude of warming events. Here we propose a robust quantitative approach for multi-proxy analysis in paleoclimate studies. To demonstrate this, we study the latest Maastrichtian warming event (LMWE) in the ODP 174AX Bass River core (New Jersey), and integrate five independent paleotemperature proxies covering the last million years of the Cretaceous. Our integrated temperature reconstruction suggests that, after a climatically stable period, a latest Cretaceous warming of 3.9 ± 1.1 °C occurred between ∼450 and 100 kyr before the K–Pg boundary. The error on this reconstructed temperature should be considered the absolute minimum error, as poorly constrained or unknown uncertainties cannot be fully propagated. The warming event was followed by a gradual cooling to pre-warming conditions towards the end of the Cretaceous. Furthermore, the record suggests multiple warming pulses during the LMWE. The results of this integrated approach are consistent with other latest Cretaceous temperature records, suggesting that the trend described here represents a global signal.

1. Introduction

Latest Cretaceous (late Maastrichtian) paleotemperature records suggest a global warming of 2–8 °C between ∼450 and ∼100 kyr before the K–Pg boundary (Li and Keller, 1998; Barrera and Savin, 1999; Olsson et al., 2002; Wilf et al., 2003; Westerhold et al., 2011; Tobin et al., 2012; Petersen et al., 2016; Thibault et al., 2016; Vellekoop et al., 2016; Barnet et al., 2017), possibly as a result of Deccan Traps volcanism (Chenet et al., 2007; Schoene et al., 2015; Henehan et al., 2016). Yet, despite these reports, the exact magnitude of the late Maastrichtian warming event (LMWE) remains poorly constrained, mainly because several sources of uncertainty are not, or are poorly, addressed.

Firstly, many, especially older, paleotemperature studies provide proxy records without an analytical error and without providing the raw data in the form of a table or supplementary data file. This introduces a source of uncertainty when using these records in further studies. Though these uncertainty estimates have been included in recent publications on late Cretaceous temperature evolution (Tobin et al., 2012, 2014; Petersen et al., 2016), their absence in older studies limits the accuracy of estimates of the magnitude of the LMWE.

Calibrations used to reconstruct past temperatures introduce a second source of uncertainty. Although they often include a regression error (e.g. Bemis et al., 1998; Lear et al., 2002; Martin et al., 2002; Anand et al., 2003; Kim et al., 2010), this does not provide a realistic estimate of their predictive capabilities as obtained by cross-validation techniques. If the raw data used in temperature calibrations are unavailable, it is impossible to correctly propagate the prediction errors associated with these calibrations, prohibiting accurate estimation of the magnitude of the LMWE. Furthermore,

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lack of access to the raw data does not permit improvement of calibrations by combining different data sets, or by redesigning calibration equations as a result of new insights.

The third source of uncertainty is of a more fundamental nature. The use of modern-day calibrations to reconstruct climatic and environmental changes in the paleo-domain introduces uncertainties whose magnitudes are poorly constrained (or even completely unknown), owing to the fact that parameters of proxy calibrations for temperature estimation cannot be verified for deep-time applications. Modern-day proxy calibrations could be based on species that were nonexistent in the late Cretaceous, and it is not known whether species in this time interval responded similarly to temperature changes as their modern-day counterparts. Detailed information on paleo-sea-water composition (salinity, oxygen isotopes, Mg/Ca ratios) is similarly unavailable. Further uncertainty on the magnitude of warming arises from proxy records (Li and Keller, 1998; Barrera and Savin, 1999; Olsson et al., 2002; Tobin et al., 2012) that may have suffered from unknown diagenetic effects (Pearson et al., 2001), which could have altered the original signal. And lastly, each single proxy may also be influenced by variables other than temperature, which prohibits reliable comparison of temperatures derived from different proxies (Lawrence and Woodard, 2017). For example, regional hydrological change as well as the waxing and waning of ice sheets, possibly even in the latest Cretaceous greenhouse climate (Miller et al., 2005), may have influenced late Maastrichtian marine $\delta^{18}O$ values and thereby reconstructed temperatures.

In addition to these three sources of uncertainty, that prohibit an accurate reconstruction of the LWME, previous late Maastrichtian multi-proxy studies compare temperature records from different locations, rather than comparing multiple proxy records from a single location (Wilf et al., 2003; Woelders et al., 2017). As a result, observed differences between temperature records in these studies could also be caused by, for instance, local diagenetic processes instead of actual (local) climate signals. Furthermore, owing to problems of age constraints (Olsson et al., 2002; Wilf et al., 2003; Woelders et al., 2017), it cannot be excluded that seemingly age-equivalent signals are actually diachronous.

Finally, the low temporal resolution (commonly <10 data points in the last million years of the Maastrichtian, Barrera and Savin, 1999; Tobin et al., 2012, 2014; Petersen et al., 2016) and low signal-to-noise ratios (Li and Keller, 1998; Barrera and Savin, 1999; Wilf et al., 2003; Westerhold et al., 2011; Petersen et al., 2016) also limit detailed reconstruction of the LMWE.

The above sources of uncertainty, and additional challenges posed by low resolution datasets and low signal-to-noise ratios, hamper a robust determination of the magnitude of the LMWE, which in turn complicates the assessment of the environmental and ecological implications of late Maastrichtian climate change on the K–Pg mass extinction.

The risks associated with relying on single proxy records may be reduced by using multiple paleo-temperature proxy records. Data in multi-proxy studies are commonly displayed side by side to highlight consistency between datasets, or to illustrate patterns of variability unique to each dataset. This approach can, however, be improved upon substantially by statistically integrating temperature records based on different proxies. This enables quantification of the signal shared by the individual datasets (cf. Bloemsma et al., 2012), and allows for more accurate and robust quantification of temperature trends and anomalies. The latter is extremely relevant for climate modeling purposes, as accurate estimates of past sea surface temperatures (SSTs) are a prerequisite for paleoclimate model forcing (e.g. Sloan et al., 2001) and model evaluation (e.g. Otto-Bliesner et al., 2017).

Here we introduce a formal approach to multi-proxy analysis based on data integration, to permit objective assessment of the significance of temperature changes. Integration of reconstructed temperature records based on different datasets using different proxies, and thus different temperature calibrations, requires quantification of the uncertainties of each, since the uncertainty directly translates to the weight of evidence of the data and temperature transfer functions. Following this approach, we present an integrated multi-proxy temperature reconstruction of the late Maastrichtian, spanning approximately the last million years of the Cretaceous, by combining benthic and planktic foraminiferal $\delta^{18}O$ and Mg/Ca and the organic geochemical SST proxy TEX_{86} records for the Bass River core (ODP Leg 174AX, New Jersey, Fig. 1) (Miller et al., 1998; Olsson et al., 2002).

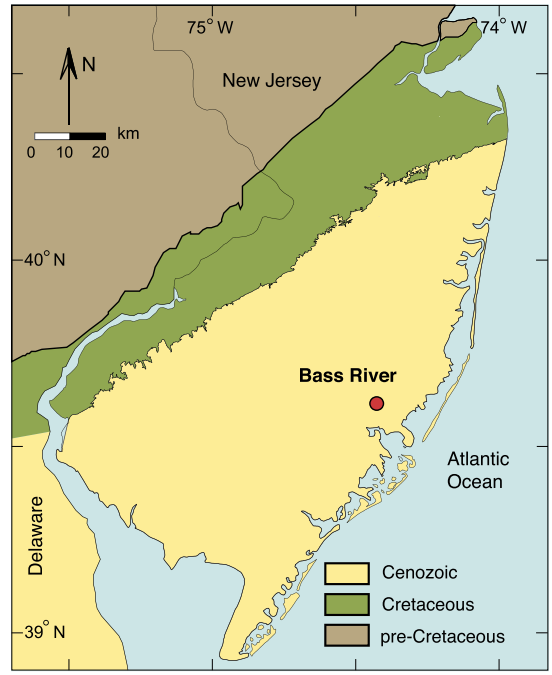

Fig. 1. Geological map of the New Jersey shelf area with the location of ODP Leg 174 AX Bass River site in New Jersey, USA, indicated. Modified after (Esmeray-Senlet et al., 2015). (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

The shelf sequence of Bass River (paleodepth ∼100 m, Olsson et al., 2002) comprises an uppermost Maastrichtian record with exceptionally well-preserved benthic and planktic foraminifera (Fig. 2) and biomarker lipids, enabling a multi-proxy temperature reconstruction. The LMWE has previously been identified in the Bass River core, based on stable oxygen isotopes (Olsson et al., 2002; Esmeray-Senlet et al., 2015), indicating that this sedimentary archive is ideal for a case study aimed at testing robust multi-proxy paleo-temperature reconstruction. The glauconite-rich sediments suggest low rates of sediment accumulation, but there is no evidence of the presence of hiatuses in this interval (Miller et al., 1998). Furthermore, despite the limited distance (∼100 km) of the Bass River site to the paleo-coastline (Esmeray-Senlet et al., 2015), the site is directly connected to the open ocean and likely experienced little terrestrial influx (Zachos et al., 2006). This suggests that the site is likely to have recorded the effects of global climate change.

2. Material and methods

2.1. Stable oxygen isotope analysis

Samples were washed over a sieve with a mesh of 63 μm and ultrasonically cleaned. Only specimens from the size fraction of 125–630 μm were analyzed. For benthic $\delta^{18}O$ analysis, duplicate