EXAMINING THE FIDELITY OF CARBON ISOTOPE RECORDS IN THE PALEOCENE-EOCENE THERMAL MAXIMUM

A Dissertation in

Geosciences

by

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Submitted in Partial Fulfilment

of the Requirements

for the Degree of

Doctor of Philosophy

December 2020
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ABSTRACT

Ocean and environmental conditions of the past are stored in sediment in “proxy records,” records that contain information about physical and chemical states of the ocean and atmosphere. Variations in sedimentation rate, bioturbation, winnowing, and dissolution modify the deep-sea sedimentary record, complicating the apparent relationship between stratigraphic depth and time of a geochemical proxy record and make it more difficult to decode past climates and environments. During the Paleocene-Eocene Thermal Maximum (PETM; 55.6 Ma) in particular, a large input of isotopically light carbon was injected into the ocean and atmosphere over a brief time interval, indicated by a negative carbon isotope excursion (CIE) and a large global warming of the atmosphere and surface ocean. The CO$_2$ released into the ocean resulted in shoaling of the calcite compensation depth (CCD) and dissolution of sea-floor carbonates. The resultant dissolution erased the onset of the PETM CIE at many locations. In order to understand how this dissolution and other processes affected the relationship between stratigraphic depth and time of geochemical proxy records, researchers have attempted to correlate PETM records at different locations.

In this dissertation, I apply a technique called dynamic time warping (DTW) to identify gaps and distortions in proxy records and correlate (in time) them at different locations during the PETM. DTW is a statistical technique for correlating records; other methods often correlate records subjectively. I first aligned the most analyzed, best preserved PETM proxy records, Ocean Drilling Program Site 690 (Maud Rise) and the Leg 208 (Walvis Ridge) depth transect of sites. DTW was also used to align preserved proxy records generated from models that simulate preservation of a PETM paleoenvironmental signal under various depositional settings. I also expanded the capabilities of DTW to employ a multivariate approach to align two proxies at
once, Fe & Ba. I concluded that DTW provides an objective way to align proxy records and rectify data loss associated with disconformities and other types of distortions, leading to a more complete understanding of the geologic record of past episodes of biotic and environmental change.

A bioturbation and dissolution model was also used to simulate the preservation of a PETM signal under various depositional settings. The preserved proxy records created from this model were compared to some of the most well-studied PETM records. Through this comparison, I gained new insights into how bioturbation and dissolution affect the preservation of PETM proxy records.

Overall, this dissertation demonstrates that DTW is an effective tool to align chemostratigraphic records from the PETM.
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ACKNOWLEDGEMENTS

I would like to thank my adviser (Dr. Lee Kump) for all of his help in completing this project, even with his numerous responsibilities as the Dean of Earth & Mineral Sciences.

I would like to thank my advising committee (Dr. Murali Haran, Dr. Elizabeth Hajek, & Dr. Timothy Bralower) for their availability throughout my time at Penn State, and willingness to provide feedback.

Thank-you to my research team (Brandon Clark, Chloe Stanton, Ben Barnes, Meng Wang, Mingsong Li, & Kalev Hantsoo) for providing personal and professional support. I would like to especially thank Mingsong Li for providing me with the Acycle code.

I am grateful to Angela Packer, Jo Ann Lehtihet, and the rest of the administrative staff for their assistance in helping me navigate through the requirements needed to graduate.

I am thankful to the Heising-Simons Foundation for providing funding through an award to Lee Kump, Sandra Kirtland Turner, and Andy Ridgwell for the project entitled “Instigating a Mechanistic Understanding of the Dynamics of the Sedimentary record (‘iMUDS’).”
Chapter 1

Introduction to the fidelity of carbon isotope records in the PETM

Paleoceanography is the study of the history of oceanic conditions in the geologic past (e.g., Berger, 1991; Broecker & Peng, 1982; Van Andel et al., 1975; Wefer et al., 1999). Understanding the history of the ocean helps researchers understand which processes contributed to climate change in the global environment (Berger, 1991; Broecker & Peng, 1982; Van Andel et al., 1975; Wefer et al., 1999). Ocean and environmental conditions in the past are recorded in physical and chemical variables (such as temperature) in sediment and ice records; these records are called “proxy” records (Henderson, 2002). Geochemical proxies are stored in inorganic or organic material buried in sediment (Higginson, 2009). Ideally, upon their death, organisms that record oceanic and atmospheric conditions sink to the ocean floor and are deposited and buried in parallel, laminated beds at a constant sedimentation rate. If sediment was deposited in this matter, time would be evenly represented in sedimentary records, and it would be easier to understand past environments. Unfortunately, sedimentary records are more complicated; different processes act to change the sedimentation rate and distort or erase proxy signals. In deep-marine settings, mineral shells from organisms that contain important environmental information can be re-mineralized before reaching the ocean floor. Only a small percentage of soft-tissue organic matter reaches the ocean floor, and a larger, yet still small proportion of mineral shells composed of CaCO$_3$ reaches the sea floor (Henson et al., 2012). Even upon reaching the ocean floor, CaCO$_3$ can then undergo dissolution, erasing important geochemical information (Morse et al., 2007), and recrystallization, mixing geochemical signals in the water column with the water chemistry conditions at the ocean floor (Henderson, 2002). Sediments in the upper few meters of the sediment column can also undergo bioturbation; burrowing
organisms mix the sediments, distorting the depth/time relationship of the proxy signal (Darwin, 1892; Meysman et al., 2006). These different processes act to create gaps and distortions in the sedimentary record, establishing a convoluted relationship between depth and time of a geochemical proxy. Proxy records of the same event often show significant differences, leading to uncertainties in climate reconstructions.

The issue of proxy preservation is particularly pronounced in records from a past global warming event, the Paleocene-Eocene Thermal Maximum (PETM). During this period, a large input of isotopically light carbon was injected into the ocean and atmosphere over a brief time interval, indicated by a negative carbon isotope excursion (CIE) of 3.5-4.5 per mil over <20 kyr (Kennett & Stott, 1991; Bralower et al., 1997), leading to an abrupt global warming of 5-8°C (Kennett & Stott, 1991; McInerney & Wing, 2011; Zachos et al., 2006) followed by a gradual recovery (130 to 190 ky) (Röhl et al., 2007; Farley & Eltgroth, 2003). The CO$_2$ released into the ocean lowered the pH and carbonate ion content of seawater. This caused a shoaling of the lysocline and calcite compensation depth resulting in dissolution of sea-floor carbonate. The dissolution of sea-floor carbonate caused much of the proxy information to be erased at the onset of the event in deep-sea sites (e.g., Bralower et al., 2014). The PETM is important to understand better because it provides an analog to understanding impacts of modern global warming and ocean acidification, and biotic change today; it shows the effects of massive carbon input to the ocean and atmosphere (Dickens 1997).

There have been a number of challenges in understanding proxy records in the PETM. Two of the most analyzed and best preserved PETM records are ODP Site 690 (Maud Rise) and the Leg 208 (Walvis Ridge) depth transect of sites (Bains et al., 1999; Zachos et al., 2004). In these records, there is still significant dissolution at the onset of PETM, erasing some of the most vital
information (Bralower et al., 2014; Zachos et al., 2005). Leg 208 has a number of cores drilled near each other, located at different depths with varying amounts of dissolution. Correlating these records help recover some of the missing information erased by dissolution. Zachos et al. (2005) attempted to correlate bulk sediment carbon isotope ($\delta^{13}$C) records from ODP Leg 208 Sites 1262, 1263, 1265, 1266, 1267, and ODP Site 690. These $\delta^{13}$C records were correlated under the assumption that during the PETM, shifts in the $\delta^{13}$C signal were globally synchronous.

Despite its general success, the method used by Zachos et al. (2005) to align the carbon isotope records at Walvis Ridge and Maud Rise is somewhat subjective and less precise. The alignment involves the selection of breaks in slope and inflection points of the $\delta^{13}$C records based on limited samples and is subject to local variability. Röhl et al. (2007) correlated records from Walvis Ridge and Maud Rise using precessional cycles in XRF core scanning data of Fe, Ba, and Ca. This is also a subjective method of alignment because the precessional cycles are manually identified.

1.1 Goals of Research

The objective of this dissertation is to explore the issue of preservation of the sedimentary record. We want to deconvolve gaps and distortions in the sedimentary record to help us better understand how these different signals vary with time and thus help us minimize uncertainty in reconstructing paleoenvironments. Accurately reconstructing paleoenvironments ultimately helps us have better constraints to improve climate models.

If we had more understanding of specific proxy records and could more accurately correlate them, we can better reconstruct the overall global $\delta^{13}$C PETM signal by combining signals from different locations. We could also create more accurate age models for sedimentary records. Dynamic time warping (DTW) is employed in this research as a tool for better understanding
In this dissertation, specifically, we want to use DTW to align synchronous parts of proxy records at different locations. By aligning a more distorted or incomplete proxy record to a more complete proxy record, we can identify missing information in an incomplete proxy record. We can also infer the environment of deposition of that particular record. Additionally, we want to investigate the fidelity of the sedimentary record by modeling bioturbation and dissolution of PETM $\delta^{13}$C records using an open-ocean model to yield further insight into how these processes affect the preservation of a signal.

In summary, our research goals are to:

- Develop DTW as a tool to align chemostratigraphic records from the PETM
- Gain new insights into the fidelity of proxy records from the PETM

I.2 Summary of Dissertation Chapters


DTW was used to identify gaps in proxy records of the Paleocene-Eocene Thermal Maximum (PETM), aligning bulk sediment carbonate isotope records ($\delta^{13}$C) from various deep-sea sediment core sections spanning the event. PETM $\delta^{13}$C records from the Walvis Ridge, South Atlantic transect of ODP Leg 208 (Sites 1262, 1263 and 1265) were specifically aligned to each other. The alignments were similar to previously published manually established alignments and consistent with the expectation that shallower sites have more complete records. The $\delta^{13}$C record from a Southern Ocean site (Maud Rise; ODP Site 690) was then aligned to ODP Site
1263, the most complete Walvis Ridge site. This alignment identifies a gap in Site 690, indicating that peak excursion $\delta^{13}C$ values were not recorded. This chapter has been published in Geochemistry, Geophysics, Geosystems, with my coauthors Dr. Lee Kump, Dr. Andy Ridgwell, Dr. Sandra Kirtland Turner, Dr. Carling C. Hay, and Dr. Timothy J. Bralower.

1.2.2: Chapter 3: Investigating the effects of bioturbation and dissolution on PETM bulk carbonate $\delta^{13}C$ records

A bioturbation model was used to evaluate how bioturbation and dissolution affect the preservation of synthetic PETM bulk carbonate $\delta^{13}C$ signals under a variety of scenarios of seafloor dissolution and mixed layer depths. The model results show that increasing bioturbation slightly decreases the magnitude of the CIE and lengthens the perceived duration of the onset. Dissolution does not begin to have a noticeable effect on the shape and magnitude of the CIE until a clay layer starts to develop, at which time gaps are created in the $\delta^{13}C$ record. Additionally, the temporary reversal in slope in bulk carbonate $\delta^{13}C$ records at Site 1263 and Site 690 are preserved when there are relatively low amounts of bioturbation and lower amounts of dissolution. These results would support the hypothesis that there were multiple injections of light carbon during the PETM, the effects of which are only preserved in some $\delta^{13}C$ records.

This chapter will be submitted to a journal with my co-authors Dr. Lee Kump and Dr. Timothy J. Bralower.

1.2.3: Chapter 4: Aligning synthetic preserved proxy records from deep-marine and fluvial-deltaic models

Deep-marine and fluvial-deltaic sedimentation models were used to create synthetic preserved proxy records from a PETM palaeoenvironmental signal under a variety of depositional
settings. Dynamic time warping (DTW) was used to align the model output records (preserved proxy records) to the model input record (complete paleoenvironmental signal) to assess the accuracy of DTW alignments under different parameter settings. Increasing bioturbation and dissolution usually decreased the accuracy of the alignment. Dissolution may only have an appreciable effect on the accuracy of the alignment if there was sufficient dissolution to create a clay layer. In fluvial-deltaic records, DTW was relatively accurate if the candidate record shows evidence of large-scale features in the target record (such as the PETM excursion).

1.2.4: Chapter 5: Expanding the capabilities of Dynamic Time warping to employ a multivariate approach

The capabilities of dynamic time warping (DTW) were expanded to employ a multivariate approach, where multiple proxies at one location can be aligned to the same proxies at another location. We aligned Ba & Fe proxies from Maud Rise & Walvis Ridge simultaneously. A multivariate alignment was performed for Site 690 and Site 1262 to Site 1263; yielding similar results to Röhl et al. (2007) alignments.
References


Chapter 2


Key Points

- Dynamic Time Warping can be employed to successfully align chemostratigraphic records.
- Dynamic Time Warping provides an objective way to align $\delta^{13}$C records of the PETM.
- The new alignments indicate gaps in sections previously considered complete, demonstrating the value of the approach.

Abstract

Variations in sedimentation rate, bioturbation, winnowing, and dissolution modify the deep-sea sedimentary record, complicating the apparent relationship between stratigraphic depth and time of a geochemical proxy record and confounding the extraction of a clear picture of past climates and environments. Dynamic time warping (DTW) is used to align time series with similar patterns. Here we explore the use of DTW to identify gaps in proxy records of the Paleocene-Eocene Thermal Maximum (PETM), aligning bulk sediment carbonate isotope records ($\delta^{13}$C) from various deep-sea sediment core sections spanning the event. Alignment of PETM $\delta^{13}$C records from the Walvis Ridge, South Atlantic transect of ODP Leg 208 (Sites 1262, 1263 and 1265) was similar to previously published manually established alignments and consistent with the expectation that shallower sites have more complete records. The $\delta^{13}$C record from a Southern Ocean site (Maud Rise; ODP Site 690) was then aligned to ODP Site 1263, the most
complete Walvis Ridge site. This alignment identifies a gap in Site 690, indicating that peak excursion $\delta^{13}C$ values were not recorded. We conclude that DTW provides an objective way to align climate proxy records and rectify data loss associated with unconformities and other types of distortions, leading to a more complete understanding of the geologic record of past episodes of biotic and environmental change.

2.1 Introduction

Geochemical proxies provide invaluable records of past environmental conditions. Skeletal and organic materials from planktic and benthic marine organisms are primary sources of geochemical proxies and ideally are deposited and buried in stratigraphic order at a constant sedimentation rate, and without subsequent modification of their chemical, mineralogical, and isotopic composition, or physical mixing of materials. In reality, a host of factors including variations in sedimentation rate, winnowing, seafloor dissolution, bioturbation, nondeposition, and other processes during early burial often generate gaps and distortion in the sedimentary record. Winnowing involves the removal, transportation and redeposition of sediments caused by flowing water, while seafloor dissolution of carbonates occurs when the carbonate ion concentration and pH of the deep ocean declines (e.g. Hönisch et al., 2012) or as a result of oxidation of organic matter during burial. Bioturbation involves the mixing of sediments by organisms at the ocean floor, causing older sediment to be brought up to the surface and newly deposited sediment to be buried deeper. All of these processes complicate the apparent relationship between depth in the sediment column and time of deposition for geochemical proxies, erasing information and impeding the correlation of records from different locations.

Accurate correlation of proxy records is important, but also difficult, particularly during episodes of rapid environmental change for which generating and aligning new records is
greatest. A pre- eminent example involves records from the Paleocene- Eocene Thermal
Maximum (PETM), 56.01±0.05 million years ago (Zeebe & Lourens, 2019). During the PETM,
$^{13}$C-depleted (‘isotopically light’) carbon was rapidly injected into the ocean and atmosphere, as
indicated by a negative carbon isotope excursion (CIE) of 3.5-4.5 ‰ over <20 kyr (Kennett &
Stott, 1991; Bralower et al., 1997), leading to an abrupt global warming of 5-8°C (Kennett &
Stott, 1991; McInerney & Wing, 2011; Zachos et al., 2006) and a gradual recovery for a total
event duration of 120 to 220 kyr (Röhl et al., 2007; Farley & Eltgroth, 2003; McInerney & Wing,
2011). The CO$_2$ sequestered in the ocean during the event lowered the pH and carbonate ion
concentration in seawater, and the resulting post-depositional dissolution of carbonate mineral
particles erased proxy information at some deep-sea sites (e.g., Zachos et al., 2005; Ridgwell,
2007a; Bralower et al., 2014a). Attaining an accurate interpretation of the PETM is important
because it provides a potential analog for the impacts of greenhouse-gas driven global climate
warming today (e.g., Dickens, 1997) and may tell us about the strength of feedbacks between
carbon cycling and a warming climate (e.g., Gutjahr et al., 2017).

Previous attempts to piece together proxy records of the PETM at high resolution have
primarily employed correlation using carbon isotope stratigraphy and astrochronology (Röhl et
al., 2007). Two classic deep-sea locations, Ocean Drilling Program (ODP) Site 690 (Maud Rise)
and ODP Leg 208 (Walvis Ridge) transect, both in the South Atlantic (Fig. 1), are considered to
provide relatively complete records of the event. However, dissolution near the base of the CIE
in the Leg 208 records scales in severity as a function of paleo-ocean depth, making it
challenging to estimate rates and extent of environmental change in this critical interval. Zachos
et al. (2005) correlated bulk sediment carbon isotope ($\delta^{13}$C) records from the Leg 208 sites using
visual matching of features in the $\delta^{13}$C records, supplemented by records of Fe content, magnetic
susceptibility, and nannofossil biostratigraphy. They also aligned the Leg 208 records to the Site 690 δ<sup>13</sup>C record to determine age, using an astronomical age model developed for Site 690 (Röhl et al., 2007). These correlations and the associated chronology have provided an influential framework for understanding the deep-sea response to the PETM carbon injection and interpretation of the nature of the event as a whole.

However, despite its general success and widespread use, the method used by Zachos et al. (2005) to align the carbon isotope records is subjective, involving the recognition of breaks in slope and inflection points in the δ<sup>13</sup>C records. Dynamic time warping (DTW) provides the means for correlating these sites in an objective fashion.

DTW, and similar dynamic programming tools, (Giorgino, 2009; Kotov & Pälike, 2018) are ideally suited for aligning records that have distortions and gaps. They have been applied in a variety of fields, including voice recognition (Levinson et al., 2013; Sakoe & Chiba, 1978), computational biology (Durbin et al. 1998; Webb et al., 2002; Zhu et al., 1998), and to a limited extent, paleoceanography and paleoclimatology (Lin et al., 2014). Alignments are accomplished by stretching or compressing the depth (or time) axis on the “candidate” record (typically the one considered to be less complete and more distorted) to find the statistically strongest correlation with the more complete or “target” record (Berndt & Clifford, 1994). The aligned candidate record is then presented on the target’s depth (or time) axis. These techniques have also previously been applied in the geosciences for the alignment of oxygen isotope records (Lisiecki & Lisiecki, 2002) and magnetic susceptibility logs (Hladil et al., 2010). Most recently, Hay et al. (2019) used DTW to create an array of possible alignments of Early Cambrian carbonate δ<sup>13</sup>C records that were both statistically significant and geologically plausible, leading to better constraints on the timing of animal diversification. Hidden Markov models (HMM) have also
been used in the alignment of oxygen isotope records with the capability of finding uncertainties in the alignment (Lin et al., 2014). This particular method has the advantage of less dependence on user-derived parameters, deriving uncertainty from the estimation of sedimentation rates.

In this study, we applied the Hay et al. (2019) script “dtw.m” for its use of generalized fitting parameters, allowing us to avoid the (over) use of subjective tie points while assessing a new method for record alignment. We applied this tool to the same bulk $\delta^{13}$C records of the PETM from ODP Sites 1262, 1263, 1265 and 690 used in Zachos et al. (2005). We show that DTW reproduces the general features of the alignments of Zachos et al. (2005), but provides an objective way to align proxy records. The technique also identifies potential gaps and sedimentation-rate variations that were not detected in the Zachos et al. (2005) alignments, showing its potential in stratigraphic correlation of complex records.

2.2 Data

Bulk sediment $\delta^{13}$C and wt. % CaCO$_3$ records from Walvis Ridge (Southeast Atlantic) and Maud Rise (Southern Ocean sector of the South Atlantic) were used in the alignments. The Walvis Ridge bulk $\delta^{13}$C records were generated using samples obtained during ODP Leg 208, which recovered pelagic carbonate ooze and claystones spanning the Paleocene-Eocene (PETM) boundary (Zachos et al., 2004). Advanced piston coring recovered multiple, vertically offset holes at five sites (1262, 1263, 1265, 1266, and 1267) between 1400 and 3500 m paleowater depth. These sites were considered relatively stratigraphically complete and undisturbed across the upper Paleocene and lowermost Eocene (Zachos et al., 2004).

The bulk carbonate $\delta^{13}$C records from Leg 208 Sites 1263, 1262, and 1265, and the wt. % CaCO$_3$ record for Sites 1262 and 1265, were obtained at sampling intervals ranging from 1 to 5 cm (available at: https://doi.pangaea.de/10.1594/PANGAEA.772042; Zachos et al., 2005; Fig 2).
At these sites, sediments change abruptly from light gray nannofossil ooze to a greyish brown ash-bearing clay at the onset of the PETM before gradually transitioning back into light grey nannofossil ooze during the peak and recovery of the event. The thickness of the clay layer generally increases with ocean depth, from 6 cm at the shallowest site (1263) to 35 cm in the deepest site (1262) (Zachos et al., 2005; Fig. 2). This relationship is consistent with the expectation that during an ocean acidification event the deepest sites would be exposed to corrosive waters the longest, with dissolution not only of newly arriving carbonate sediment but also “burn down” into the pre-existing latest Paleocene sediments. Site 1265 is a notable exception to this trend. The wt. % CaCO$_3$ record from Site 1265 does not decrease to 0 wt. % and the clay layer is the thinnest (even though Site 1265 was in deeper water than Site 1263). However, because the other sites show thick clay layers, it is likely that either uppermost Paleocene carbonate was bioturbated into the basal PETM, or the earliest part of the event may be missing in this section (Zachos et al., 2004).

Sediments from Maud Rise were collected during ODP Leg 113 (Barker & Kennett, 1988) at Site 690 where the PETM isotope excursion was first identified by Kennett and Stott (1991). Site 690 records were some of the first used to determine the duration of the PETM through both orbital chronology (Röhl et al., 2000) and $^3$He measurements (Farley & Eltgroth, 2003). The PETM paleo-water depth of this site was approximately 2100 m. Unlike the Leg 208 records, Site 690 maintains a relatively high CaCO$_3$ content throughout the PETM (Farley & Eltgroth, 2003; Fig. 2). There is no clay layer and little visual evidence of significant dissolution. Bulk carbonate $\delta^{13}$C data from Site 690 were obtained from Bains et al. (1999), who sampled the working half of the core at 5 cm intervals (Fig. 2). The wt. % CaCO$_3$ record for Site 690 was
from the archive half of the core at varying intervals ranging from 1 cm to 10 cm (Farley & Eltgroth, 2003). The data are available at: https://doi.pangaea.de/10.1594/PANGAEA.723912.

2.3 Methods

In DTW, alignments are performed between two records at a time: a target record and a candidate record. The target record is presumed to be a relatively complete and continuous record (depth series) of the interval of interest. The candidate record is a depth series from another site covering a similar time interval. The candidate record is initially considered as less complete.

The squared difference is calculated between each value in the candidate and target records, using either raw or normalized values of the time series. For the alignment between Site 690 and Site 1263, the records were first standardized to a mean of 0 and a standard deviation of 1 to accommodate the possibility that the true magnitude of the excursion at these two sites differed. In contrast, within the two Walvis Ridge transect records, this standardization was not performed because the sites were in close proximity to each other and the CIE is expected to originally have had the same magnitude (the supply of settling CaCO$_3$ to the sites was the same). An example array of squared differences – here between Sites 1262 and 1263 – is shown in Fig. 3. There are ‘N’ number of data points in the candidate series, and ‘M’ number of data points in the target series; ‘n’ refers to the column number and ‘m’ refers to the row number in the matrix.

In the Hay et al. (2019) DTW script, two “penalty” factors can be applied to the difference matrix ‘d’: the edge parameter (edge) and the diagonal parameter (g). Edge reflects the presumed extent to which the two data series span the same epoch, and g controls the amount of allowable change in relative sedimentation rates. We explored a range of $g$ (0.6 — 1.3) and edge (0.1 — 2) parameter values (Supplemental Information Section 1). We found that for these
time series, optimal fits were not improved by applying penalty factors, and we accordingly set the $g$ and $edge$ parameters equal to the default values of 1; i.e., we did not apply penalties. Alignments with alternate $g$ and $edge$ parameter values are shown in the Supplemental Information Section 1.

The minimum cumulative distance path (or warping path) ‘w’ is the path through the ‘d’ matrix that corresponds to the lowest total sum of ‘d’; the value of each grid point that the warping path is drawn through is added, and the path is chosen that minimizes this overall sum. The path begins at the top right corner in the matrix (Fig. 3). Because the data are referenced to depth, the diagonal dashed line corresponds to an alignment path with a constant relative sedimentation rate between the two records. This dynamic alignment programming method has been employed in other studies (Sakoe & Chiba, 1978; Clark, 1985; Lisiecki & Lisiecki, 2002).

Two objective criteria are used to evaluate how well the warped candidate record is aligned to the target records: the cross-correlation and the overlap. The cross-correlation evaluates the similarity between the aligned and target series by calculating their dot product at zero lag. Computation of the cross-correlation requires using only the target and aligned data that are assigned to the same depths (within a prescribed depth increment). Therefore, to measure a cross-correlation, some data points may have to be omitted from each of the data series. The overlap is the number of data points in the aligned record that were evaluated in the cross-correlation divided by the total number of data points in the original candidate record.

Data points are omitted from the cross-correlation calculation for multiple reasons. For example, in the aligned records, there are often multiple data points that have been assigned to the same depth. To calculate the cross-correlation in such a circumstance, the data must be averaged to obtain one corresponding carbon isotope value for that depth. This results in a lower
overlap value, because only one data point is calculated in the cross-correlation although it represents multiple data points. Both a high overlap and high cross-correlation indicate a good alignment with a good choice of the target series. A low overlap with a high cross-correlation indicates that the assigned target may be less complete than the candidate record, and a low cross-correlation regardless of overlap always indicates a poor alignment. For this reason, the ‘best alignment’ maximizes both cross-correlation and overlap.

The statistical significance of these Walvis Ridge transect and Site 690 alignments was evaluated by assessing the distribution of cross-correlation values produced by alignments of synthetic (random) candidate records (Site 1262, Site 1265, and Site 690) to the Site 1263 target record. One hundred thousand synthetic random-walk sequences were created using a Monte Carlo method (Haam & Huybers, 2010; Hay et al., 2019). Each of these synthetic sequences had the same number of data points as the candidate records. Each sequence was aligned to Site 1263 yielding a distribution of 100,000 cross-correlation values. The cross-correlation of the alignment of the actual candidate record to Site 1263 was compared to this distribution. The p-value is the proportion of cross-correlation values that are equal or higher in the distribution of alignments of synthetic sequences to Site 1263. A low p-value of 0.004 for the cross-correlation output from the alignment of Site 690 to Site 1263, for example, indicates that there is a 0.4% chance that a synthetic sequence could produce an equal or higher cross-correlation alignment; therefore, the alignment is significant.

2.4 Results

Table 1 reports statistics on the carbon isotope alignments between the warped and candidate records. For all of the alignments, the overlap values are higher when Site 1263 is the target record. Figures 4-6 show the alignments of Site 1262, Site 1265, and Site 690 to the target
record, Site 1263. Also shown are data obtained from Zachos et al. (2005) that show how the alignment from their study correspond with our alignments. A composite of all the deep-sea δ\(^{13}\)C alignments was created (Fig. 7); the y-axis is on an age scale, obtained from a Site 1263 age model from Röhl et al. (2007). CaCO\(_3\) records align as a consequence of the δ\(^{13}\)C DTW alignment (Fig. 8). Further analysis of how age models can be applied to the alignments is discussed in the Supplemental Information Section 3.

Each of these alignments produced p values less than or equal to 0.057, indicating high confidence that the alignments are significant. The distribution of cross-correlations produced by alignment of the synthetic records to the target record are shown in the Supplemental Information Section 2.

### 2.5 Discussion

The good agreement between Site 1263 and Site 1265 alignments (Fig. 4) was expected because Site 1263 and Site 1265 are in close proximity and at comparable water depth (1400 m paleowater depth for Site 1263 and 1850 m paleowater depth for Site 1265; Abels et al., 2016; Zachos et al., 2004) and hence are expected to have experienced a similar degree of distortion due to changing carbonate preservation across the event. Site 1263 and Site 1262 (Fig. 5) have lower cross-correlation values and overlap because Site 1263 and Site 1262 sediments were deposited at significantly different paleowater depths (1400 m paleowater depth for Site 1263 and 3600 m paleowater depth for Site 1262) (Zachos et al. 2005). Site 1263 and Site 690 have high cross-correlation but moderately low overlap values.

The overlap values within the excursion interval are consistently higher when Site 1263 is the target record (Table 1). This is expected amongst the Leg 208 records, where Site 1263 is the most complete record, but unexpected when aligned with Site 690, given that the wt. %
CaCO$_3$ records (Fig. 2) would indicate that Site 1263 underwent more dissolution than Site 690. However, the Site 690 excursion interval does reveal lower carbonate contents than the pre-excursion values; a reduction from 90 wt. % CaCO$_3$ to 60 wt. % (Fig. 2). If this reduction in carbonate content was driven by dissolution alone it would represent an additional (compared to prior to the event) 80% loss in the fraction of CaCO$_3$ delivered to the seafloor that is preserved. Moderate bioturbation could be masking even more severe dissolution (Bralower et al., 2014b).

The alignments also suggest a gap in Site 690 from Site 1263-aligned depths of 335.13 mcd to 335.29 mcd (169.96-170.01 mbsf in the original 690 record; Fig. 6), which, if real, indicates that the minimum bulk $\delta^{13}C$ excursion values might not have been recorded at Site 690 (Bains et al., 1999, Fig. 2). Core photos from Site 690 do not show any obvious change in sedimentology that would make this gap readily identifiable (see Fig. S13). Importantly, the identified gap lies stratigraphically above (later in time than) most of the major events identified from isotope, sedimentological, and micropaleontological datasets. Key environmental and biotic events, summarized by Bralower et al., 2014, cluster between 170.8 and 170.6 mbsf, almost half a meter deeper than the DTW-identified gap. The first evidence of chemical erosion occurs at 170.788 mbsf, indicated by decreasing wt% CaCO$_3$, while an increase in foraminiferal fragmentation at 170.6 mbsf suggests enhanced deep water dissolution. CaCO$_3$ content had also begun to recover and was nearly at pre-event levels by ~170 mbsf. Based on the cyclostratigraphic age model for ODP Site 690, this gap lies within the third precession cycle following the PETM onset (see Fig. S13). The gap though does occur at the nadir of the bulk CIE, and also marks the beginning of a significant stepwise reduction in Fe content (Fig. S13). McCarren et al. (2008) similarly concluded that minimum $\delta^{13}C$ excursion values were not recorded at Site 690 by benthic foraminifera, and attributed this to ecological absence. They also
concluded that the Site 1263 record is truncated by dissolution; it has a lower magnitude CIE (3‰ in the bulk record) than terrestrial carbon isotope records (up to 5 to 6‰) (McCarren et al., 2008).

Comparison of our alignment to Zachos et al. (2005) reveals a general agreement for Site 1265 (Fig. 4) and Site 690 alignments (Fig. 6) to Site 1263. The Site 1262 alignment agrees moderately well with our alignment; however, Zachos et al. (2005) inserts a longer gap in the Site 1262 record (warped to Site 1263 at 335.65 mcd; pre-warping depth of 139.98 mcd) reflecting the observed thick clay layer in which carbonate sediment is not preserved after the onset (Fig. 5). Zeebe & Lourens (2019) hypothesized a similar gap in Site 1262 in creating an astronomical time scale for Site 1262. In this case, the Zachos et al. (2005) correlation, informed by additional geological data (carbonate content), may be presenting a more accurate alignment of these two records during the onset interval.

Despite the success of the specific example presented here, DTW alignment of paleoproxy records involves a unique (as compared to more ‘traditional’ DTW usage) set of caveats and potential pitfalls. Firstly, DTW assumes monotonicity in the target record. Reworking by large-scale geologic processes such as turbidite flows and slumping are relatively easy to identify. Furthermore, deep sea sites selected for the development of high-resolution geochemical records are generally chosen to avoid such occurrences as far as possible. On a much smaller scale, bioturbation, the displacement of particles in the upper sediment column due to the feeding, burrowing, and locomotion activities of animals, has the potential to break the assumption of monotonicity. For bulk (isotope) records, as employed here, this may not be a particularly significant concern as the effect of bioturbation on bulk sediment composition is generally to smear out (reduce in amplitude) and introduce a lag into a signal rather than
stratigraphically invert signals. However, single foraminifera-based proxy records have a much greater potential for signal artifacts to be introduced (e.g., see Kirtland-Turner et al., 2017) and break the assumption of monotonicity.

There is also the question of the extent to which any two proxy records directly reflect the same primary (e.g., global) signal. Attempting to align a pair of records, one of which is not as distorted as compared to the first, but also has been significantly overprinted by a second and different signal, would obviously be problematic. For instance, in the case of a carbon isotope ($\delta^{13}C$) signal recorded in pelagic carbonate, a number of factors might act to cause the $\delta^{13}C$ signal delivered to the surface sediment to diverge (and before post-depositional distortion such as by bioturbation or changing rates of dissolution have occurred) from location to location.

These effects can be divided into factors that control how the $\delta^{13}C$ of seawater dissolved inorganic carbon (DIC) is incorporated into pelagic carbon, and those that control the $\delta^{13}C$ of DIC itself. The former group includes vital effects and for bulk carbonate records, the proportion of CaCO$_3$ derived from calcifying phytoplankton (e.g. coccolithophores) vs. calcifying zooplankton (foraminifera) (and indeed changing assemblage composition within the phytoplankton and zooplankton communities).

Primary controls on the $\delta^{13}C$ of DIC include biological productivity and air-sea gas exchange (including temperature) (Schmittner et al., 2013). While many of these controls might have a relatively predictable response to an environmental perturbation such as associated with the PETM carbon isotope excursion (e.g. using numerical models such as in Gutjahr et al., 2017), the response need not be linear, meaning the inflection points of the primary $\delta^{13}C$ signal at two different ocean locations might differ in time, yet be forced to align under DTW. However, the spatial impact of all these factors together only imparts only a 0.6‰ total variability at the
modern ocean surface (Schmittner et al., 2013), suggesting that for most paleo $\delta^{13}$C events of interest, the global signal component will be dominant. Similar arguments can be made for benthic records, but with potential changes in deep ocean circulation patterns that lead to an overprinting of any global $\delta^{13}$C signal being the greatest concern.

2.6 Conclusions and Perspectives

We found that carrying out proxy-record alignments using DTW yielded new insights into the relative completeness of two classic PETM records from Walvis Ridge in the South Atlantic Ocean and Maud Rise in the Southern Ocean. DTW results generally agree with the Zachos et al. (2005) alignments of Site 1262 to Site 1263 and Site 1265 to Site 1263. DTW indicates that Site 1263 is more complete than Site 690 within the carbon isotope excursion interval; the overlap is greater when Site 1263 is the target record and Site 690 is the candidate record. The alignment of Site 690 to Site 1263 also identifies a gap in Site 690, indicating that the Site 690 bulk carbonate record may not have preserved the minimum excursion value. Dissolution may have impacted Site 690 to a greater degree than previously thought (Bralower et al., 2014a). Alternatively, Site 690 may simply have experienced a lower magnitude CIE. We cannot confidently discriminate between these two alternatives based on our DTW results. From a more practical perspective, we found that DTW was largely able to reproduce the correlations established by expert, but non-automated and more subjective means.

However, there remain a number of uncertainties surrounding the application of DTW to deep-sea proxy records, particularly with regard to how bioturbation distorts records and the occurrence of significantly increased carbonate dissolution and hence reduced sediment rates (and even ‘erosion’) during the peak of past carbon release events such as the PETM, and how
these may affect alignment between records. We are addressing this in several lines of on-going work.

1. Our ongoing efforts are directed at developing a multivariate application of DTW to allow simultaneous alignment of multiple proxies (e.g., XRF-derived Fe and Ca, δ^{18}O, and δ^{13}C). We also are exploring the use of HMM-Match (Lin et al., 2014) for deep-time alignments because of its ability to assess uncertainty in alignments. The apparent inability of DTW to align the Site 1262 and Site 1263 records during the interval of intense dissolution at the PETM onset may be addressed through application of HMM-Match to these records, using He accumulation data to better constrain sedimentation rates.

2. We aim to employ an Earth system model that gives us the capability of creating ‘synthetic’ (‘artificial’) deep-sea proxy records that encapsulate the key distorting features of proxy records such as changes in carbonate preservation (including ‘erosion’) and bioturbation (Ridgwell, 2007a,b) together with a background orbital variability. In being able to generate both ‘perfect’/complete records as well as records of varying distortion and incompleteness, and for simulated events of different characteristics, we will be in a position to develop a comprehensive empirical based understanding of the specific limitations of DTW for aligning paleo proxy records, and identify the characteristic events and depositional environments in which DTW can be fully relied upon.
Acknowledgements

This study was funded by a Heising-Simons Foundation award to Kump, Kirtland Turner, and Ridgwell for the project entitled “Instigating a Mechanistic Understanding of the Dynamics of the Sedimentary record (‘iMUDS’).” We thank Linda Hinnov and two anonymous reviewers for their constructive suggestions on an earlier version of the manuscript. Datasets for this research are available in these in-text data citation references: Zachos et al. (2005) (with data available at: https://doi.pangaea.de/10.1594/PANGAEA.772042), Farley & Eltgroth (2003) (with data available at: https://doi.pangaea.de/10.1594/PANGAEA.723912) and Bains et al. (1999). The dynamic programming Matlab script is available at the GSA Data Repository item 2019175, available online at https://www.geosociety.org/datarepository/2019/.

References


Table 1: Cross-correlation and overlap values for all carbon isotope DTW alignments performed with $g=1$ and $edge=1$. 

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<th>edge</th>
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Figure 1: 56.0 Ma reconstruction showing the locations of Maud Rise (ODP Site 690) and Walvis Ridge (ODP Leg 208 Sites 1262, 1265, and 1263). Map from http://www.odsn.de. References shown for paleowater depths: ¹Barker and Kennett (1988), ²Kennett and Stott (1991), ³Zachos et al. (2004), and ⁴Zachos et al. (2005),

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Figure 2: Bulk carbonate $\delta^{13}$C (black lines), from ODP Site 690B (Bains et al., 1999) plotted versus meters below the sea floor (mbsf), and CaCO$_3$ (wt %; gray lines) from Farley and Eltgroth (2003). Sites 1262A, 1263 C/D, and 1265A (Zachos et al., 2005) plotted versus meters composite depth (mcd). CaCO$_3$ wt% for Sites 1262, 1263, and 1265 from Zachos et al. (2005). Shaded region corresponds to clay layer. Figure adapted from Zachos et al. (2005). vPDB stands for Vienna PeeDee Belemnite.
Figure 3: Squared difference map between two normalized proxy records. Target record is Site 1263 carbon isotope record (in red); candidate record is an interpolated Site 1262 carbon isotope record (in black). In this example, both records have been normalized to a mean value of zero and scaled by standard deviations from that mean. The warping path is the solid black line in central panel of the figure. The dashed diagonal line is an example of an alignment path with a constant relative sedimentation rate. The left panel shows the alignment of the candidate record (in black) with the target record (in red). Gaps in the candidate record correspond to vertical sections of the warping path; clumping of the candidate record corresponds to horizontal sections of the warping path reflecting relatively high sedimentation rate relative to the target.
Figure 4: Bulk carbonate $\delta^{13}$C record of Site 1265 aligned to Site 1263. Also shown is the alignment from Zachos et al. (2005). The statistical significance assessment of the alignment yielded a $p$-value of 0.000.
Figure 5: Bulk carbonate $\delta^{13}$C record of Site 1262 aligned to Site 1263. Also shown is the alignment from Zachos et al. (2005). The statistical significance assessment of the alignment yielded a p-value of 0.057.
Figure 6: Bulk carbonate $\delta^{13}C$ record of Site 690 aligned to Site 1263. Both records have been normalized to a mean of zero and scaled by standard deviations from that mean (positive and negative). Also shown is the alignment from Zachos et al. (2005). The statistical significance assessment of the alignment yielded a p-value of 0.004.
Figure 7: All alignments for δ^{13}C to Site 1263. Age based on Röhl et al. (2007) Site 1263 age model.
Figure 8: All alignments for CaCO$_3$ to Site 1263. Age based on Röhl et al. (2007) Site 1263 age model. The DTW alignment was conducted on the $\delta^{13}$C records, this figure shows how CaCO$_3$ aligns as a consequence. Bulk carbonate CaCO$_3$ data from Site 690 (Farley and Eltgroth 2003) were sampled from the archive half and bulk carbonate $\delta^{13}$C data from Site 690 (Bains et al. 1999) were sampled from the working half of Site 690. The archive half of the core likely sampled a burrow, which created a 7-cm offset between the PETM onset between the archive half and working half (Bralower et al., 2014b). Therefore Site 690 CaCO$_3$ depths could not be aligned accurately to the Site 690 $\delta^{13}$C depths and Site 690 CaCO$_3$ data was not shown in this figure.
Chapter 3

Investigating the effects of bioturbation and dissolution on PETM bulk carbonate $\delta^{13}$C records

Abstract

Deep-sea bulk carbonate $\delta^{13}$C records from the Paleocene-Eocene Thermal Maximum (PETM) can differ significantly in the shape and magnitude of the carbon isotope excursion (CIE). At Site 690 and Site 1263, for instance, there is an initial negative CIE followed by a slight temporary reversal in slope, then by a final negative excursion. In other deep-sea bulk carbonate $\delta^{13}$C records, for example, Sites 1001 and 1265, there is just one constant negative CIE. In this study, we attempted to explain the differences seen in bulk carbonate PETM $\delta^{13}$C records. We used a bioturbation model to evaluate how bioturbation and dissolution affect the preservation of synthetic PETM bulk carbonate $\delta^{13}$C signals under a variety of scenarios of seafloor dissolution and mixed layer depths. The model results show that increasing bioturbation slightly decreases the magnitude of the CIE and lengthens the perceived duration of the onset. Dissolution does not begin to have a noticeable effect on the shape and magnitude of the CIE until a clay layer starts to develop, at which time gaps are created in the $\delta^{13}$C record. Additionally, the temporary reversal in slope in bulk carbonate $\delta^{13}$C records at Site 1263 and Site 690 is preserved under low amounts of bioturbation and relatively lower amounts of dissolution. These results would support the hypothesis that there were multiple injections of light carbon during the PETM, the effects of which are only preserved in some $\delta^{13}$C records.
3.1 Introduction

During the Paleocene-Eocene Thermal Maximum (PETM), 55.8 million years ago, thousands of petagrams of isotopically light carbon were injected into the ocean-atmosphere system over less than 20,000 years (Dickens et al. 1995; Panchuk et al., 2008; McInerney & Wing, 2011). The release of isotopically light carbon resulted in a negative shift in the $\delta^{13}$C of the ocean as recorded in benthic and planktic foraminifera and bulk carbonate (Fig. 1) (Kennett & Stott, 1991; Thomas & Shackleton, 1996). The carbon isotope excursion (CIE) coincided with rapid warming (4-5°C) at the onset of the PETM (Kennett & Stott, 1991; Dunkley-Jones et al., 2013; Frieling et al., 2017). The magnitude of the CIE is important in understanding the source and amount of carbon released (e.g. Pagani et al., 2006b, Panchuk et al., 2008; Zeebe et al., 2009; Cui et al., 2011; Turner & Ridgwell, 2016). Different processes affect the preservation of the CIE signal in marine sediment. Bioturbation is the process by which organisms at the sea floor mix sediments; older sediment is brought to the surface and newer sediment is buried more deeply (e.g., Guinasso & Schink, 1975; Darwin 1892; Meysman et al., 2006). Dissolution through exposure to corrosive (calcite-undersaturated) deep waters removes carbonate as it settles to the seafloor and is buried, and persistent exposure to corrosive waters (“burn down”) can lead to the establishment of a “clay layer” dominated by insoluble detrital clay minerals, completely devoid of carbonate (Berger & Heath, 1968; Broecker & Peng, 1982; Henson et al., 2012; Morse et al., 2007; Walker & Kasting, 1992). Carbonate dissolution increases rapidly at depths equivalent to the lysocline and almost complete dissolution occurs at sites below the CCD (Berger & Heath, 1968; Berger & Winterer, 1974). As a result, deeper sites tend to have undergone more dissolution (e.g., Murray & Renard, 1891).
There are differences between the magnitude of the CIE found in marine and in terrestrial sections. Out of 117 marine records and 48 terrestrial records of the CIE, marine records have a median CIE of -2.6 ‰ and terrestrial records have a median CIE of -4.6 ‰ (McInerney & Wing 2011). Some have attributed these differences in magnitude to amplification of the CIE in the terrestrial records due to carbon cycle processes (e.g., Bowen et al., 2004; Pagani et al., 2006a, 2006b; Schouten et al., 2007; Smith et al., 2007). McCarren et al. (2008) hypothesized that the differences in magnitude are more attributable to truncation of the CIE in marine records, due to severe dissolution of marine carbonates and damping by bioturbation (Pagani et al., 2006b; Zachos et al., 2005; Zeebe & Zachos, 2007). This hypothesis would assume that terrestrial sections more accurately record the CIE and thus are a more reliable recorder of the light carbon released into the atmosphere. However, the carbon isotope values of terrestrial plants are influenced by various environmental factors, such as water availability and plant type (Bowen et al., 2004; Diefendorf et al., 2010). Additionally, marine δ13C records can be derived from different sediment components that record the isotope signal differently, including bulk carbonate, benthic foraminifera, planktic foraminifera, organic matter, and others. Carbon cycle modeling shows that a light carbon injection into the ocean surface system, such as during the PETM, should result in a larger magnitude CIE in organic matter than in carbonate material (Kump & Arthur, 1999). Based on 11 bulk organic matter records for the PETM and 33 bulk carbonate records, the median marine PETM CIE magnitude in bulk organic matter records is significantly greater than the bulk carbonate records (-3.5 ‰ vs -2.4 ‰) (McInerney & Wing, 2011). There are similar median CIE magnitudes for the PETM for bulk carbonate (-2.4 ‰), planktic foraminifera (-2.6 ‰), and benthic foraminifera (-2.6 ‰) records (McInerney & Wing, 2011). Bulk carbonate records are used more often in analysis, however, since they are more
often higher resolution and can be obtained quicker than single or multi foraminiferal specimen samples, and only require small sample volumes to obtain data (Hain et al., 2014). Foraminifera are also more prone to dissolution and recrystallization (Reghellin et al., 2015). Bulk carbonate records are dominated by coccoliths, sometimes comprising greater than 90% of the bulk record (Stoll, 2005). Coccoliths can have up to a 5% array of interspecific vital effects or shifts in stable isotope fractionations; changing coccolith assemblages could create significant artifacts in bulk records (Bralower, 2002; Paull & Thierstein, 1987; Thomas et al., 2002; Ziveri et al., 2003).

Some of the most heavily studied PETM sections have significant differences in the shape of the bulk carbonate CIE. Interesting features appear at Site 690 (Fig. 1A), Site 1215 (Fig. 1D), and Site 1263 (Fig. 1E). Site 1263 shows an initial negative CIE followed by a temporary reversal in slope, then a slight negative excursion, another reversal in slope, followed by a final negative excursion (335.44-335.68 mcd). Site 690 and Site 1215 also show an initial negative CIE then by a slight temporary reversal in slope, followed by a final negative excursion (170.5-170.7 mbsf and 54.3-54.4 m respectively). Site 1209 shows some evidence of this feature as well, but only based on one data point at 216.4 mcd. Bains et al. (1999) suggests that the δ¹³C record at Site 690 shows evidence for multiple injections of isotopically light carbon separated by intervals in which the carbon cycle was in stasis. Ajayi et al. (2020) used dynamic time warping to align Site 690 and Site 1263, and found that this temporary reversal in slope in the bulk carbonate record occurs at the same time in both records. Frieling et al. (2017) posits that there was an initial input of ¹³C-depleted carbon at the onset of the PETM, followed by additional carbon release within the PETM. They hypothesized that the carbon input came from intrusive volcanism in the North Atlantic region. Carbon release of thermogenic methane from a hydrothermal vent postdated the onset of the PETM, and could have caused the additional carbon
injection after the onset of the PETM. However, these features in Site 690, Site 1215, and Site 1263 could be an artifact of the higher resolution in bulk carbonate records, since this temporary reversal in slope doesn’t appear in foraminifera records. These features could also be created by changing coccolith assemblages during the PETM onset, an interval where there is more dissolution (Bralower, 2002; Stoll 2005).

A number of other studies have similarly modeled bioturbation in ocean sediments (Berger & Heath, 1968; Shull, 2001; Boudreau et al., 2001; Choi et al., 2002; Turner et al. 2017, Trauth, 1998; Hull et al., 2011; Trauth, 2013). Most of the current models create sediment records with a bulk (average) composition of particles and over-simplify sediment-mixing processes. A number of these models track individual particles during the mixing process (Shull, 2001; Trauth, 1998; Trauth, 2013; Hull et al., 2011). A bioturbation model that tracks individual particles has the potential to track ‘true’ age (age of deposition) of each individual particle to create age models for bioturbated records. In future work, particle tracking models can be used to compare the difference between single species records and bulk records from the same location. One of the advantages of a few of these models, including TURBO2, is that the distribution of particles is transformed in a ‘transition’ matrix (Shull, 2001, Trauth 1998, Trauth, 2013). Tracking individual particles in a ‘transition matrix’ provides the potential for particles to be mixed based on a probability that a given particle in one layer would move to another. This allows flexibility in imposing different constraints on the extent of bioturbation. Hull et al (2011), in contrast, use a random walk approach, material is mixed between given layers stochastically. An advantage of using TURBO2 (Trauth, 2013), specifically, is accessibility; it uses MATLAB, is computationally inexpensive, and is publicly available.
In this study, we evaluated how bioturbation and dissolution affects the preservation of idealized carbon isotope signals by using TURBO2 to simulate these processes. We imposed a variety of scenarios of seafloor dissolution and mixed layer depth and compared the δ¹³C profiles generated by the model to bulk δ¹³C profiles from well-studied deep-sea sites. Our objective was to see how varying the degree of bioturbation and dissolution of a PETM δ¹³C record (Fig. 2) could yield further insight into how bioturbation and dissolution affect preservation of the signal. Two different idealized PETM δ¹³C records were created; one was generated in this study, using PETM duration estimates based on astronomical cyclostratigraphy and extraterrestrial ³He fluxes summarized by McInerney & Wing (2011) (Fig. 2A), and the other was a smoothed Site 1263 δ¹³C record (Fig. 2B), the most expanded and highest magnitude deep-sea CIE. We compared these model outputs to PETM bulk carbonate δ¹³C records from different locations to see if TURBO2 was able to reproduce features seen in these records. By using the Site 1263 δ¹³C record as an input, we can determine if the other records at Walvis Ridge can be simulated by modeling bioturbation and dissolution; and if the temporary reversal in slope in the CIE likely reflects a signal throughout the ocean-atmosphere system as opposed to a localized feature.

3.2 Data & Methods

TURBO2 applies bioturbation and dissolution to an input signal, in our case the PETM bulk carbonate δ¹³C record (Fig. 2). We used two different δ¹³C input signals. The first was generated in this study, using PETM duration estimates from McInerney & Wing (2011) (Fig. 2A). The synthetic δ¹³C record was created with a CIE of 3.5 ‰, corresponding to a presumed complete marine bulk carbonate CIE if there was no bioturbation or dissolution (McInerney & Wing, 2011; McCarren et al., 2008). The synthetic record was created in time, with a duration of 300 kyr. The onset interval of the excursion, from the beginning of the excursion to the minimum
value, in continental sections ranges from 8-23 kyr (Aziz et al., 2008; Bowen et al, 2001; Magioncalda et al., 2004; McInerney & Wing, 2011). The duration of the onset cannot be reliably derived from deep-sea sections, due to dissolution at the onset of the PETM (McInerney & Wing, 2011). For our synthetic record, we selected a higher-end estimate of 20 kyr for the onset duration (e.g., Cui et al., 2011). The body and the recovery of the CIE totaled 195 kyr, based on $^{3}$He calibration of rates at ODP Site 1266 on Walvis Ridge (Murphy et al. 2010). The body and recovery totaled 171 kyr for Site 1266 when time calibration was performed using orbital cyclostratigraphy (Röhl et al., 2007). A more recent orbital chronology on a terrestrial $\delta^{13}$C record in the Big Horn Basin found that the PETM duration totaled ~200 kyr (Westerhold et al., 2018). In our synthetic record created in this study, we rounded to allocate 200 kyr for the maximum CIE value to recover back to the original $\delta^{13}$C value. The second $\delta^{13}$C record (Fig. 2B) was adapted from the $\delta^{13}$C record at Site 1263 (Zachos et al., 2004), likely the most expanded and complete deep-sea record. It was smoothed using a seven-point running average and displayed on the same time axis shown in (Fig. 2B) with a data point every 1 kyr.

In our TURBO2 code, four variables are input to the program: age, number of mixed layers, abundance of particles, and isotope signature. The age corresponds to the age column of the synthetic record (Fig. 2). For a given input matrix, there is a data point (or a layer) every 1 kyr. The number of mixed layers determines how many layers (or matrix rows) are being mixed. If the record is in age and the sedimentation rate is 1cm/kyr, for a mixed layer of 10, the mixed layer depth is 10 cm. The pre-onset sedimentation rate for the PETM in deep-sea records ranged broadly from 0.3 cm/kyr-2.3 cm/kyr (Bralower et al., 2014; Röhl et al., 2007, Westerhold et al., 2007, Westerhold et al., 2008). This sedimentation rate decreases during the PETM interval, largely due to dissolution of the carbonate sediment. A constant sedimentation rate of 1cm/kyr
was applied to convert the number of mixed layers to a mixed layer depth for the first synthetic record (Fig. 2A & Fig. 2B). The mixed layers were varied from a value of 0, 10, and 20, which corresponds to mixed layer depths of 0 cm, 10 cm, and 20 cm, respectively; an average bioturbation depth in deep-sea sediment is about 10 cm with a standard deviation of 5 cm (Boudreau, 1998). The abundance of particles varies between five settings; low dissolution, moderate dissolution, high dissolution/instantaneous recovery, high dissolution/intermediate recovery, and high dissolution/delayed recovery (Fig. 2). These ‘abundance of particles’ profiles correspond to the number of CaCO$_3$ particles that reach the sediment-water interface and are deposited. A low dissolution corresponds to 90,000 CaCO$_3$ particles reaching the sediment-water interface throughout the 300 kyr interval. This dissolution profile would be an idealized perfectly preserved record, with no dissolution. The overall preservation percentage is 100%, meaning all of the record is preserved. A moderate dissolution corresponds to an initial deposition of 90,000 CaCO$_3$ particles followed by a sharp decrease (coinciding with the CIE), where only 50,000 CaCO$_3$ particles are deposited, followed by a gradual recovery to 90,000 CaCO$_3$ particles being deposited. This dissolution profile is comparable to the Site 690 CaCO$_3$ wt.% profile (Fig. 3), where the CaCO$_3$ profile decreases, with a quick recovery to the initial wt.% values. The overall preservation percentage is 86%, meaning 86% of the record was preserved after dissolution. All of the high dissolution profiles begin with 90,000 CaCO$_3$ particles being deposited, followed by a sharp drop off to zero CaCO$_3$ particles being deposited. The recovery back to 90,000 CaCO$_3$ particles varies from delayed to instantaneous recovery, as seen in Figure 2. Although, the total number of particles in a bulk carbonate record is much higher, likely tens of millions, once the number of particles in the model is exceeded, the model results do not change, so 90,000 particles represents a sufficiently high enough number of particles. These three high dissolution
profiles are comparable to the Site 1262, Site 1265, and Site 1263 CaCO$_3$ wt.% profiles (Fig. 3), where the wt.% values drop to zero, and begin to recover back to the initial wt. % values either instantaneously, or after a period of time. The preservation percentage for the high dissolution profiles is 68% when the recovery is instantaneous, 64% when the recovery is intermediate, and 59% when the recovery is delayed. The isotope signature in the input correspond to the isotope values of the synthetic record at each depth or time recorded (every 1 kyr) (Fig. 2).

The final output results for the first synthetic record are converted to depth based on the changing sedimentation rate derived from the dissolution of CaCO$_3$. The model always has a pre-onset sedimentation rate of 1 cm/kyr. In our model, this sedimentation rate corresponds to an initial deposition of 90,000 particles of CaCO$_3$ and 10,000 particles of clay. Therefore, a sedimentation rate of 1 cm/kyr corresponds to 100,000 total particles of sediment being deposited every thousand years. As the number of CaCO$_3$ particles decreases due to dissolution, the sedimentation rate also decreases. If the CaCO$_3$ particle deposition decreases to 50,000 particles, under the assumption that the clay sedimentation remains constant, 10,000 particles of clay are still being deposited. Therefore, there would be a sedimentation of 60,000 particles of sediment being deposited every thousand years, or 0.6 cm/kyr. If the CaCO$_3$ particle deposition decreases to 0 particles of CaCO$_3$, there would be 0 particles of CaCO$_3$ deposited and 10,000 particles of clay being deposited. There would be 10,000 particles of sediment being deposited every thousand years, a sedimentation rate of 0.1 cm/kyr.

3.3 Results

A compilation of all of the final $\delta^{13}$C records in depth are shown in Fig. 4 with varying dissolution profiles and mixed layer depths. Mixed layer depth increases from top to bottom, and dissolution increases from left to right. As shown in previous work, dissolution and bioturbation
can reduce the magnitude of the CIE (McCarren et al., 2008). As dissolution intensity increases, more of the record is erased, corresponding to an increasingly thicker clay interval. The peak of the CIE is also not preserved (Figs. 4D, 4E, 4I, 4J, 4N, & 4O). Increasing mixed layer depth results in a smaller magnitude CIE, with the pre-PETM values being decreased and the peak CIE values being increased. The peak CIE shifts to a shallower depth and the onset of the PETM is shifted to a deeper depth and decreases more gradually, resulting in a perceived longer PETM onset. Both increased mixed layer depth and increased dissolution intensity results in an even larger gap (thicker clay interval), with more of the record before and after the peak of the CIE being erased. The results show that increasing bioturbation both decreases the magnitude of the CIE and lengthens the onset of the PETM. Increasing dissolution intensity creates gaps in the record, erasing the peak of the CIE and CaCO$_3$ before and after the peak.

A high dissolution intensity also has a larger overall effect on altering the record than high amounts of bioturbation. In the profile for high dissolution/delayed recovery and 0 cm mixed layer depth (Fig. 4E) there is a greater amount of alteration of the record than the low dissolution and 20 cm mixed layer depth profile (Fig. 4K). However, the effects of dissolution intensity are not as pronounced in the record until the dissolution intensity is high with an intermediate to delayed recovery (Fig. 4D, 4E, 4I, 4J, 4N, and 4O). Until high dissolution is reached and remains high for a duration of time, bioturbation has a larger effect on changing the record. High dissolution with intermediate to delayed recovery corresponds to a clay layer in a bulk carbonate record. Therefore, until a clay layer forms in a bulk carbonate record where no CaCO$_3$ is deposited for a duration of time, dissolution will have a lesser effect on the record, and the $\delta^{13}$C signal is more influenced by bioturbation. Dissolution and bioturbation combined create
the most change in the $\delta^{13}$C signal, as bioturbation enhances the degradation created by high amounts of dissolution.

An assemblage of all the final $\delta^{13}$C records in time are shown in Fig. 5. As dissolution increases, decreasing carbonate results in slower sedimentation concurrent with the peak of the CIE. Consequentially, dissolution of the peak of the CIE in depth can conceal the amount of time missing from the record, either due to syn-depositional or burndown dissolution. Syn-depositional dissolution is the dissolution of newly deposited carbonate and burndown dissolution is the dissolution of previously deposited layers (Bralower et al., 2014). In other words, the thickness of a clay layer does not fully portray the time represented.

Fig. 6 shows the assemblage of all the output $\delta^{13}$C records after varying dissolution profiles and mixed layer depths were applied to the smoothed average of the Site 1263 $\delta^{13}$C record (Fig. 2B). Mixed layer depth increases from top to bottom and dissolution increases from left to right. As previously seen in Figs. 4 and 5, a clay layer begins to appear once dissolution intensity begins to increase to high dissolution/intermediate recovery and high dissolution/delayed recovery (Fig. 6D, 6E, 6I, 6J, 6N & 6O). This clay layer is large enough to erase part of the temporary reversal in slope in the middle of the CIE (Fig. 6D & Fig. 6E). Increased bioturbation, shifts the CIE slightly downwards and shifts the peak upwards. Moderate to high bioturbation, (Figs. 6F-6J) also erases the temporary reversal in slope of the CIE.

### 3.4 Discussion

A number of bulk $\delta^{13}$C records from various locations and environments were compiled (Table 1 & Fig. 1). Table 1 shows the amount of dissolution, bioturbation and magnitude of the CIE for various deep-sea PETM records; it also shows which TURBO2-generated profile (Figs.
4, 5, & 6) should match up with a given site (in the right-most column of Table 1), based on its amount of bioturbation and dissolution. For the TURBO2-generated profiles, the magnitude of the excursion roughly decreased with increasing amount of dissolution (Fig. 7) For the compiled deep-sea PETM records, the dissolution at each site was categorized based on the accompanying CaCO₃ wt % data. Surprisingly, the magnitude of the excursion roughly increased with increasing amount of dissolution (Fig. 8). The excursion magnitude is influenced by many other factors in addition to dissolution, such as biological productivity, air-sea gas exchange, and composition of the bulk carbonate, that affect the δ¹³C magnitude at different locations (Broecker, 1982; Schmittner et al., 2013). However, for the sites that were categorized as high dissolution with either intermediate or delayed recovery (Fig. 1B, 1F, 1G, 1H, & 1I) we postulate that gaps at the onset of the PETM (that are difficult to identify because they constitute such little depth) actually represent much more time than it would seem. These records are even less complete than they appear to be. Records such as Site 690, Site 1215, & Site 1263 are presumably the most complete, since they have either moderate dissolution (Site 690), or high dissolution with an instantaneous recovery (Site 1215 & Site 1263). Even though Site 1209 has low dissolution, it is not presumed to be one of the most complete records, since the site is condensed.

The Leg 208 transect on Walvis Ridge in the South Atlantic (Fig. 1E-1I) provide further confirmation of how dissolution degrades records. Along the transect, dissolution increases as the paleo-water depth increases from 1500 (Site 1263) to 3600 m (Site 1262) and the clay layer increasing from 6 to 35 cm (Zachos et al., 2005). With a general increase in dissolution one would also expect the magnitude of the CIE to decrease. This mostly happens, with the CIE ranging from 3 ‰ in Site 1263 and to 2.4 ‰ in Site 1262 (Table 2). However, Site 1266 has an
anomalously low CIE of 2.2 ‰, even though it is shallower than Site 1262. The trend seen in the Leg 208 Records, with generally a lower magnitude CIE with increasing dissolution, reflects the result seen in our study where increasing dissolution lowers the magnitude of the CIE. Additionally, Zachos et al. (2005) also found that the gaps represented by the clay layer represent larger intervals of time than they appear to at face value, with the peak CIE values most likely not reached in these records.

Site 690 and Site 1263 (Fig. 1A & 1E) represent two of the most well-studied, and most robust deep-sea records. Site 690, located at Maud Rise in the Southern Ocean sector of the South Atlantic, recorded a CIE of 2.1 ‰ (Bains et al., 1999). Site 1263 recorded a CIE of 3 ‰. There has been debate over which of these records more faithfully preserve the PETM paleoenvironmental signal (Kelly, 2002; Röhl et al., 2007). Site 1263 shows more evidence of dissolution, with a 6 cm thick clay layer. Site 690 had less dissolution, with the CaCO$_3$ wt % only decreasing to about 60%, and no clay layer developed. However, Site 690 has evidence for significant bioturbation which combined with winnowing has the potential to mix foraminiferal specimens by up to 20 cm upward or downward from their original positions (Bralower et al. 2014). In contrast, Leg 208 sites (Site 1263, 1262, 1265, 1266, and 1267) underwent limited bioturbation (Bralower et al., 2014; Zachos et al., 2004). In our study, large degrees of bioturbation more effectively degrade the record than dissolution, until a certain threshold of dissolution is reached. Once a clay layer begins to appear, the effects of dissolution begin to exceed the effects of bioturbation. If the clay layer of 6 cm for Site 1263 is sufficiently small, we could postulate that the Site 1263 record is more well-preserved than Site 690. However, since Site 1263 has a thin clay layer, we cannot state this conclusively. Site 1209 is expected to be the
best preserved; it has low dissolution and limited bioturbation (Bralower et al., 2014), although the record is very condensed because of the low sedimentation rate (Westerhold et al., 2008).

Among the PETM records compiled, 3 of the 10 preserve the temporary reversal in slope observed at Site 1263 and used as our second CIE input signal: Site 690 (Fig. 1A), Site 1215 (Fig. 1D) and Site 1263 itself (Fig. 1E). The TURBO2 outputs in Fig. 6 show that if the temporary reversal in slope in the CIE reflects a signal throughout the ocean-atmosphere system, there must be minimal bioturbation and there can’t be a large clay layer in order for the entire interval to be preserved (dissolution must be either low, moderate, or high with an instantaneous recovery). Site 690 has a CaCO$_3$ wt.% profile comparable to our moderate dissolution profile, and moderate bioturbation, Site 1209 has a CaCO$_3$ wt.% profile comparable to our low dissolution profile and low bioturbation, Site 1215 has a CaCO$_3$ wt.% profile comparable to our high dissolution/instantaneous recovery profile, and Site 1263 has a CaCO$_3$ wt.% profile comparable to our high dissolution/instantaneous recovery profile with low bioturbation (Bains et al., 1999; Bralower et al., 2014). Out of these four records, it was expected that Site 1215 and Site 1263 would preserve the temporary reversal in slope because they have low bioturbation and sufficiently low amounts of dissolution. It is surprising that Site 690 preserved this feature because it has moderate bioturbation. Site 1209 likely only partially preserved this feature because of how condensed the record is (Westerhold et al., 2008). All of the other records that do not have a temporary reversal in slope (Site 1001, Site 1265, Site 1266, Site 1267, and Site 1262) have CaCO$_3$ wt.% profiles comparable to our high dissolution with intermediate or delayed recovery profiles, and thus have a larger clay layer. One would not expect that any of these records would preserve the temporary reversal due to dissolution, so the expectation holds true.
Our results lend further credence to the hypothesis of Bains et al. (1999) and Frieling et al. (2017) that there is evidence for multiple injections of light carbon. A number of other studies have also posited that there were multiple releases of carbon (Bowen et al., 2014; Secord et al., 2010; Sluijs et al., 2006). Big Horn Basin terrestrial δ^{13}C records, which are considered to be very well-preserved, show that the beginning of the PETM has two distinct carbon release events, between which there was a recovery to background values. This suggest that there were multiple reservoirs capable of repeated carbon release (Bowen et al., 2014). Our study supports the hypotheses that this repeated carbon release came from hydrothermal vent system after the initial PETM onset (Frieling et al., 2017).

3.5 Conclusions

The model results for both input δ^{13}C records show that increasing bioturbation slightly decreases the magnitude of the CIE and lengthens the perceived duration of the onset. Dissolution also does not begin to have a noticeable effect on the record until a clay layer starts to develop. When the smoothed Site 1263 δ^{13}C record is used as the input, the temporary reversal in slope in the middle of the CIE is only preserved with low bioturbation and no clay layer. Our study supports the hypothesis that there were multiple injections of light carbon during the PETM that are only preserved in some δ^{13}C records. Future work, can modify TURBO2 to model bioturbation and dissolution on bulk records with changing species assemblages to see if the temporary reversal in slope can be reproduced and under which conditions.
References


Table 1: Extent of dissolution, bioturbation, CIE, and corresponding TURBO2 profile for various deep-sea PETM sites. *Site 1215 affected by drilling disturbance. ¹Bralower et al. (2014); ²Sigurdsson et al. (1998); ³Lyle et al. (2002)
Figure 1: Compilation of deep-sea bulk carbonate records during the PETM. A. Site 690 (Bains et al., 1999) B. Site 1001 (Bralower et al., 1997) C. Site 1209 (Colosimo et al., 2005) D. Site 1215 (Leon-Rodriguez & Dickens, 2010) E. Site 1263 (Zachos et al., 2004) F. Site 1265 (Zachos et al., 2004) G. Site 1266 (Zachos et al., 2004) H. Site 1267 (Zachos et al., 2004) I. Site 1262 (Zachos et al., 2004)
Figure 2: Bulk carbonate $\delta^{13}C$ and CaCO$_3$ abundance profiles to be modeled in TURBO2. $\delta^{13}C$ profile in red. Various profiles of CaCO$_3$ abundance in gray scale. Starting with high dissolution/delayed recovery (40,500 particles of clay dissolved/kyr) in black, then high dissolution/intermediate recovery (36,200 particles of clay dissolved/kyr), high dissolution/instantaneous recovery (31,800 particles of clay dissolved/kyr), moderate dissolution (14,100 particles of clay dissolved/kyr), and then low dissolution (0 particles of clay dissolved/kyr) in the lightest gray color. Figure 1A is a synthetic PETM $\delta^{13}C$ record in time and Figure 1B is a smoothed version of Site 1263 $\delta^{13}C$ record displayed in time.
Figure 3: Bulk carbonate $\delta^{13}$C (black lines), from ODP Site 690B (Bains et al., 1999) plotted versus meters below the sea floor (mbsf), and CaCO$_3$ (wt% ; gray lines) from Farley and Eltgroth (2003). Sites 1262A, 1263 C/D, and 1265A (Zachos et al., 2005) plotted versus meters composite depth (mcd). CaCO$_3$ wt% for Sites 1262, 1263, and 1265 from Zachos et al. (2005). Shaded region corresponds to clay layer. Figure adapted from Zachos et al. (2005) and Ajayi et al. (2020). vPDB stands for Vienna PeeDee Belemnite.
Figure 4: TURBO2 results in depth of varying mixed layer depths and abundance profiles applied to the synthetic PETM δ¹³C profile. Original record in black, and TURBO2 output in red. Clay layer in gray. From top to bottom row: bioturbation low (0 cm mixed layer), moderate (10 cm mixed layer), high (20 cm mixed layer). From left to right: low dissolution (100% preservation), moderate dissolution (86% preservation), high dissolution/instantaneous recovery.
(68% preservation), high dissolution/intermediate recovery (64% preservation), high dissolution/delayed recovery (59% preservation)
Figure 5: TURBO2 results in time of varying mixed layer depths and abundance profiles applied to the synthetic PETM $\delta^{13}$C profile. Original record in black, and TURBO2 output in red. Clay layer in gray. From top to bottom row: bioturbation low (0 cm mixed layer), moderate (10 cm mixed layer), high (20 cm mixed layer). From left to right: low dissolution (100% preservation), moderate dissolution (86% preservation), high dissolution/instantaneous recovery (68% preservation).
preservation), high dissolution/intermediate recovery (64% preservation), high dissolution/delayed recovery (59% preservation)
Figure 6: TURBO2 results in time of varying mixed layer depths and abundance profiles applied to the smoothed Site 1263 δ¹³C profile. Original record in black, and TURBO2 output in red. Clay layer in gray. From top to bottom row: bioturbation low (0 cm mixed layer), moderate (10 cm mixed layer), high (20 cm mixed layer). From left to right: low dissolution (100% preservation), moderate dissolution (86% preservation), high dissolution/instantaneous recovery (68% preservation), high dissolution/intermediate recovery (64% preservation), high dissolution/delayed recovery (59% preservation)
Figure 7: Magnitude of CIE compared to the amount of dissolution for TURBO2 results in depth of varying mixed layer depths and abundance profiles applied to the synthetic PETM $\delta^{13}$C profile.
Figure 8: Magnitude of CIE compared to the amount of dissolution for 9 deep-sea sites compiled in Table 1 and Figure 1.
Chapter 4

Investigating the effects of bioturbation and dissolution on PETM bulk carbonate δ¹³C records

Abstract

In both deep-marine and fluvial-deltaic environments, a variety of processes create gaps and distortions in the sedimentary record, establishing a convoluted relationship between depth and time of a geochemical proxy. Here deep-marine and fluvial-deltaic sedimentation models are used to create synthetic preserved proxy records under a variety of depositional settings from a PETM paleoenvironmental signal in an effort to deconvolve the records. Dynamic time warping (DTW) is used to align the model output records (preserved proxy records) to the model input record (complete paleoenvironmental signal). Our objective is to test the accuracy of DTW under a range of depositional settings. Because the correct placement of the output record relative to the input record is already known from the model, we can assess how accurately DTW aligns the output record back to the input record. Additionally, we investigate how different DTW parameter settings affect the accuracy of the alignments under different depositional settings. Bioturbation, and for carbonate sediments, dissolution decrease the accuracy of the alignment. The effects of dissolution scale with severity and duration, and are particularly notable when dissolution creates a clay layer, as in many deep-sea PETM records. In fluvial-deltaic records, DTW was relatively accurate if the candidate record shows evidence of large-scale features in the target record (for instance the PETM carbon isotope excursion).
4.1 Introduction

A variety of processes affect how geochemical proxies preserve paleoenvironmental signals in different depositional environments. In deep-marine environments, mineral shells from organisms that contain important environmental information (“proxy records”) can be re-mineralized before reaching the sea floor. Only a small percentage of soft-tissue organic matter reaches the ocean floor, and a larger, yet still small proportion of mineral shells composed of CaCO$_3$ reaches the ocean floor (Henson et al., 2012). Even upon reaching the sea floor, CaCO$_3$, can then undergo dissolution, erasing important geochemical information (Morse et al., 2007), and recrystallization, mixing geochemical signals in the water column with the water chemistry conditions at and below the ocean floor (Henderson, 2002). Sediments in the upper few meters of the column can also undergo bioturbation; burrowing organisms mix the sediments, distorting the depth/time relationship of the proxy signal (Darwin, 1892; Meysman et al., 2006). In fluvial-deltaic environments, sedimentation rates are significantly faster than in deep-marine environments. Fluvial-deltaic sedimentation rates range from 10cm/kyr to 30 cm/kyr (Trampush & Hajek, 2017); deep-sea sedimentation rates range from 0.01cm/yr to 3cm/yr (Lyle, 2016). With such high rates of sedimentation, bioturbation and dissolution are less of a factor in mixing and removing sediment. In fluvial-deltaic environments, episodic deposition of sediments can be driven by small events such as channel avulsions, or larger events such as floods and storms (Trampush & Hajek, 2017). These events of episodic deposition are often concentrated into specific areas. As a result, stratigraphic sections close to each other geographically can be vastly different and have variable degrees of completeness (Ganti et al., 2011; Straub et al., 2012). However, one of the advantages of studying fluvial-deltaic records is that multiple records in
close proximity to each other can recreate a complete paleoenvironmental signal (Trampush & Hajek, 2017).

It is important to deconvolve gaps and distortions in the sedimentary record to facilitate paleoenvironmental reconstruction and to be able to correlate proxy records accurately to understand how these different signals vary in both space and time. Accurately reconstructing paleoenvironments ultimately helps us have better constraints to improve climate models. DTW, introduced in Chapter 1, was used to correlate $\delta^{13}$C signals in Walvis Ridge and Maud Rise records, the most robust proxy records from the Paleocene-Eocene Thermal Maximum (PETM). During the PETM, isotopically light carbon was injected into the ocean and atmosphere, indicated by a negative carbon isotope excursion (CIE) coinciding with a rapid warming of the ocean and atmosphere at the onset of the PETM (Kennett & Stott, 1991). In this chapter, we test the effectiveness of DTW by correlating records generated from two different sedimentation models that simulate the process of preservation of a paleoenvironmental signal during the PETM. One of the models, the TURBO2 model (Trauth, 2013), simulates preservation of a PETM signal in a deep-sea environment and the other, the Trampush & Hajek (2017) model, simulates preservation of a signal in a fluvial-deltaic environment. In both models, an input record (representing a complete paleoenvironmental signal) is run through the model under different preservation settings to yield a number of output records (representing preserved proxy records). DTW is used to align the output records (preserved proxy records) to the input record (complete paleoenvironmental signal). Our objective is to test the accuracy of DTW under a range of depositional settings. A deep-sea sedimentation model and a fluival-deltaic sedimentation model were specifically compared in order to investigate the differences between how DTW aligns the output records to the input records in two different settings. In both models,
only a proportion of the complete paleonenvironmental signal is preserved, with various intervals of gaps in the record. In the deep-sea model, most of the gaps in the record are concentrated at the PETM excursion, because of increased dissolution during that interval. In the fluvial-deltaic model, gaps occur randomly throughout the record, since deposition and erosion in fluvial-deltaic settings are more episodic. Because the correct placement of the output record relative to the input record is already known from the model, we can assess how accurately DTW aligns the output record back to the input record. Knowing the accuracy of DTW alignments in different depositional environments from modeled proxy records can help us estimate the uncertainty of DTW alignments in different depositional environments from observed proxy records. Additionally, we investigate how different DTW parameter settings affect the accuracy of the alignments under different depositional settings.

4.2 Challenges using DTW for Proxy Records

Hay et al. (2019) initially used the DTW code adopted here and in Chapter 2 to align Cambrian $\delta^{13}$C$_{\text{carb}}$ records from the Anti-Atlas mountains in Morocco. The “target” record was radiometrically dated, and the two candidate records were not. Possible alignments were found between the candidate records and the target record. Hay et al. (2019) used two parameters to constrain the warping path: the diagonal parameter ($g$) and the edge parameter (edge). Edge reflects the presumed extent to which the two data series span the same epoch, and $g$ controls the amount of allowable change in relative sedimentation rates. A value of $g>1$ increases the penalty assigned to the warping path when gaps or intervals of compression are created in the candidate record. In other words, values of $g>1$ are assigned when the candidate record and the target record are thought to have relatively constant relative sedimentation rate (there are no gaps assigned to the candidate record and the warping path is linear and diagonal). A value of $g<1$
decreases the penalty assigned to the warping path when gaps or intervals of compression are created in the candidate record. In other words, values of $g < 1$ are assigned when the candidate record and the target record are thought to have time-varying relative sedimentation rates (there are more likely large gaps in the candidate record or intervals of compression, and the warping path deviates from linear). When $g = 1$ there can be both gaps and intervals of compression inserted into the candidate record; but the code does not constrain these to be created. A value of $edge > 1$ is assigned when it is thought that the starting point and end point of the candidate record and the target record occur at the same time. A value of $edge < 1$ is assigned when it is thought that the start point and end point of the candidate record and the target record occur at different times. Hay et al. (2019) tested a range of $g$ and $edge$ values ($g$ ranging from 0.98 to 1.01 and $edge$ ranging from 0.1 to 0.15) to find a range of possible alignments of the candidate record to the target record. They used a number of additional geological constraints to influence which $g$ and $edge$ values were picked.

If there is no a priori knowledge or geological constraints that give insight into how the candidate record should align to the target record, picking specific $g$ and $edge$ values will be challenging, and changing $g$ and/or $edge$ can create very different alignments. In such a case, one must rely on two outputs produced from the code: overlap & cross-correlation to determine what combination of $g$ and $edge$ most likely provides the best alignment (as outlined in Chapter 2). The cross-correlation evaluates the similarity between the aligned and target series by calculating their dot product at zero lag. Computation of the cross-correlation requires using only the target and aligned data that are assigned to the same depths (within a prescribed depth increment). Therefore, to measure a cross-correlation, some data points may have to be omitted from each of the data series. The overlap is the number of data points in the aligned record that
were evaluated in the *cross-correlation* divided by the total number of data points in the original candidate record. With no other geological information to constrain the alignment, *cross-correlation* and *overlap* should be the most accurate predictor of how well a warped record aligns to a target record. Our hypothesis in Chapter 2 was that maximizing both *cross-correlation* and *overlap* would yield the best possible alignment.

### 4.3 Methods

Here we test this hypothesis on output records from two models: a fluvial-deltaic and a deep-sea sediment model. In each of these models, a complete paleoenvironmental signal is input into the model. The model then distorts and erases part of that original signal, to create an output record. DTW is then performed on the output record to align it back to the original complete paleoenvironmental signal. DTW is run multiple times to align each output record (candidate record) to input record (target record) over a range of $g$ and $edge$ values, with each run yielding a different alignment. Each depth (or time) value in the candidate record is aligned to the target record to generate a “warped” depth (or time). Since the warped record (or output record) is generated from the target record (or input record) in either the fluvial-deltaic or open-ocean model, we also know the “correct” depth (or time) and could test how accurate the alignment was. A mean absolute error (MAE) is obtained for each DTW alignment to assess the alignment’s accuracy. The MAE is the total sum of the absolute values of the differences between the “correct” depth (or time) and the “warping” depth (or time) for each data point in the proxy record divided by the total number of values. In other words, the MAE is the average difference between the “correct” depth (or time) and “warped” depth (or time) in a given alignment.
**Mean Absolute Error** = \( \sum_{i=1}^{n} \frac{|\text{correct depth (or time)} - \text{warped depth(or time)}|}{\text{total number of values}} \)

More accurate alignments have a smaller MAE. For each DTW run, *cross-correlation*, *overlap*, and MAE values are calculated. After a range of \( g \) and *edge* values are tested, a plot depicting the *cross-correlation*, *overlap*, and MAE is created with each data point depicting the *cross-correlation*, *overlap*, and MAE for one model run with a specific \( g \) and *edge* value (Fig. 1). In this plot, we also indicate the model run that minimizes the MAE (in red in Fig. 1). According to our hypothesis the minimum MAE value should be in the top right corner of Fig. 1. Fig. 1 depicts four different example alignments with various \( g \) and *edge* values tested.

We first applied DTW to align records from a stochastic sedimentation model simulating fluvial-deltaic conditions. Trampush & Hajek (2017) created this model to simulate the preservation of proxy signals during the Paleocene-Eocene Thermal Maximum (PETM). An input proxy signal was created which mimicked the behavior of a \( \delta^{13} \)C signal over 350 kyr that spans the PETM and Eocene Thermal Maximum-2 carbon isotope excursions (Fig. 2). Randomized noise was added to this input proxy signal. A distribution of the possible annual sedimentation rates was then created (Fig. 3A) that dictates how the input proxy signal was sampled. For each given year, there was either sedimentation, non-deposition, or erosion, based on whether the annual sedimentation was positive, zero, or negative. The distribution was centered at an expected long-term sedimentation rate of either 10 cm/kyr or 30 cm/kyr. A large deposition event of 4 m in a given year or a large erosion event of -4 m in a given year could happen when an infrequent event such as a large flood or storm occurs (Trampush & Hajek, 2017). This probability distribution was drawn from once a year for 350,000 years to build up a sedimentary record (Fig. 3B). In Fig. 3B, the gray areas show the parts of the record that have
been eroded, and the colored areas show the parts of the record that were preserved. The proxy value assigned to each year corresponds to the proxy value in the complete record in Fig. 2 for that given year. Four different models were created with different parameters for the distribution in Fig. 3A. A given model had either a high sedimentation rate, with the distribution centered at 30 cm/kyr, or a low sedimentation rate, with the distribution centered at 10 cm/kyr. A model also either had high variability, with the largest allowable annual sedimentation or erosion at ±4 m, or low variability, with the largest allowable annual sedimentation or erosion at ±2 m.

Table 1: Trampush & Hajek (2017) model input settings

<table>
<thead>
<tr>
<th>Model</th>
<th>Median Sedimentation Rate</th>
<th>Variability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1</td>
<td>High (30 cm/kyr)</td>
<td>Low (maximum annual event = ±2 m)</td>
</tr>
<tr>
<td>Model 2</td>
<td>High (30 cm/kyr)</td>
<td>High (maximum annual event = ±4 m)</td>
</tr>
<tr>
<td>Model 3</td>
<td>Low (10 cm/kyr)</td>
<td>Low (maximum annual event = ±2 m)</td>
</tr>
<tr>
<td>Model 4</td>
<td>Low (10 cm/kyr)</td>
<td>High (maximum annual event = ±4 m)</td>
</tr>
</tbody>
</table>

Trampush & Hajek (2017) created synthetic records from each of the four models. They found that 100% of Model 1 (high sedimentation rate/low variability) output records preserved the large PETM excursion, 88% of Model 2 (high sedimentation rate/high variability) records preserved it, 87% of Model 3 (low sedimentation rate/low variability) records preserved it, and 69% of Model 4 (low sedimentation rate/high variability) records preserved it. Fig. 4 shows examples of some of the output records Trampush & Hajek (2017) created from each model.

We also applied DTW to align records from the TURBO2 model used in Chapter 2 to evaluate how bioturbation and dissolution affect the preservation of PETM bulk carbonate δ¹³C signals under a variety of scenarios of seafloor dissolution and mixed layer depths. The input bulk carbonate δ¹³C signal is shown in Fig. 5. Simulations of preservation of this input signal under a variety of settings were performed (Table 2).
Fig. 6 shows the compilation of output records generated from the TURBO2 model run on an original synthetic PETM record. In this figure, mixed layer depth increases from top to bottom, and dissolution increases from left to right. The output record is in red and the input signal is in black.

Table 2: TURBO2 model input settings

<table>
<thead>
<tr>
<th>Amount of Dissolution</th>
<th>Amount of Bioturbation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>Low</td>
</tr>
<tr>
<td>Low</td>
<td>Medium</td>
</tr>
<tr>
<td>Low</td>
<td>High</td>
</tr>
<tr>
<td>Moderate</td>
<td>Low</td>
</tr>
<tr>
<td>Moderate</td>
<td>Medium</td>
</tr>
<tr>
<td>Moderate</td>
<td>High</td>
</tr>
<tr>
<td>High/Fast Recovery</td>
<td>Low</td>
</tr>
<tr>
<td>High/Fast Recovery</td>
<td>Medium</td>
</tr>
<tr>
<td>High/Fast Recovery</td>
<td>High</td>
</tr>
<tr>
<td>High/Moderate Recovery</td>
<td>Low</td>
</tr>
<tr>
<td>High/Moderate Recovery</td>
<td>Medium</td>
</tr>
<tr>
<td>High/Moderate Recovery</td>
<td>High</td>
</tr>
<tr>
<td>High/Slow Recovery</td>
<td>Low</td>
</tr>
<tr>
<td>High/Slow Recovery</td>
<td>Medium</td>
</tr>
<tr>
<td>High/Slow Recovery</td>
<td>High</td>
</tr>
</tbody>
</table>

For both the TURBO2 and the Trampush & Hajek (2017) models, all of the model output records were aligned back to the input signals. There were 93 total alignments for the four different sedimentation model settings in Trampush & Hajek (2017) models. 24 output records from Model 1 were aligned back to the input record, 25 output records from Model 2 were aligned back to the input record, 23 output records from Model 3 were aligned back to the input record, and 21 output records from Model 4 were aligned back to the input record. For each of the 93 alignments, a range of $g$ values, ranging from 0.1 to 2 at intervals of 0.1 and $edge$ values, ranging from 0.7 to 1.2 at intervals of 0.1 were tested. The $g$ and $edge$ values were found that...
minimized the MAE. There were 15 total output records (Fig. 6) from the TURBO2 model that were aligned back to the input proxy record. For each of these 15 alignments, a range of $g$ and \textit{edge} parameters (0.1-2 for both $g$ and \textit{edge}) were tested. The $g$ and \textit{edge} values that created the alignments with the minimum MAE were also obtained for each of the 108 alignments (93 alignments from the Trampush & Hajek (2017) model and 15 alignments from the TURBO2 model).

We also assessed whether each alignment that minimized the MAE also maximized cross-correlation and overlap by using a metric called $xc^*$overlap percentile. We multiplied the cross-correlation by the overlap for each $g$ and \textit{edge} run for a given alignment, and assessed what percentile the cross-correlation and overlap fell into for the $g$ and \textit{edge} value that minimized the MAE. For example, if the $xc^*$overlap percentile is 50\% for a given $g$ and \textit{edge} run, half of the $g$ and \textit{edge} runs have a lower $xc^*$overlap. The higher the $xc^*$overlap percentile value, the closer the run is to maximizing cross-correlation and overlap.

\textbf{4.4 Results}

For the Trampush & Hajek (2017) model, we found that in most cases, the alignments that minimized the MAE (the most accurate alignments) were those that also maximized the \textit{cross-correlation} and \textit{overlap}: of 93 alignments of the output proxy record to the input signal, the median $xc^*$overlap percentile equals 93.5\%. In other words, for an average run, the $g$ and \textit{edge} value that yielded the most accurate alignment had a higher $xc^*$overlap value than 93.5\% of the other $g$ and \textit{edge} runs. Additionally, better preserved output records were more likely to maximize the \textit{cross-correlation} and \textit{overlap} (Table 3); the $xc^*$overlap percentile is higher for better preserved models.
Table 3: Results of aligning output record from Trampush & Hajek (2017) model back to the input signal (after finding the $g$ and edge values that minimized the MAE)

<table>
<thead>
<tr>
<th>Model</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>% of output records that preserved PETM excursion</td>
<td>100</td>
<td>88</td>
<td>87</td>
<td>69</td>
</tr>
<tr>
<td>Median MAE</td>
<td>10,500 yr</td>
<td>19,000 yr</td>
<td>18,300 yr</td>
<td>20,200 yr</td>
</tr>
<tr>
<td>Median xc*overlap percentile</td>
<td>97</td>
<td>92</td>
<td>92</td>
<td>77</td>
</tr>
</tbody>
</table>

The median MAE was greater for less-well-preserved models (although Model 3 has a slightly lower median MAE than Model 2). Fig. 7 shows an alignment with the median MAE for Models 1-4. Most of the differences between the “correct” and “warped” time are small (less than 10,000 yr). Fig. 7A shows an alignment with very small error for most of the data points, but some of the data points have large errors (greater than 50,000 yr). Model 2 (Fig. 7B) & Model 3 (Fig. 7C) have somewhat larger errors than Model 1 (Fig. 7A). Model 4 (Fig. 7D) has a significantly larger MAE, with much of the larger magnitude areas of the CIE not preserved in sediment.

Fig. 8A shows the distribution of $g$ in each of the alignments performed that minimized the MAE. Out of all the alignments, 74% of the alignments have a $g=1$ when the MAE is minimized. When $g=1$, the xc*overlap percentile is 97%, meaning cross-correlation and overlap are relatively maximized. When $g<1$, out of 10 alignments the median xc*overlap percentile is 50%. When $g>1$, out of 14 alignments the median xc*overlap percentile is 51%. This shows that any time $g$ deviates from 1, and there is a forced constraint on the warping path, maximizing cross-correlation and overlap no longer creates the most accurate alignments. With $g<1$, constraints are imposed on the warping path that increases the likelihood that large gaps or intervals of compression are added to the warping path. These constraints, however, decrease the
accuracy of these alignments. There is a large range of edge values constrained by the record (Fig. 8B). Unlike the g parameter, the edge parameter that maximizes the cross-correlation and overlap did not help predict the most accurate alignment.

Fig. 9 shows the MAE distribution of the most accurate alignment (the alignment that minimizes MAE over a range of g and edge values) for each DTW alignment in each of the four models. Most of the alignments have a MAE below 20,000 yr. However, for three of the alignments (Fig. 9C & Fig. 9D), even when the cross-correlation and overlap are maximized, DTW yields MAE values greater than 80,000 yr in three cases. In each of these three examples, the only values preserved were at the beginning and the end of the record, before and after the PETM excursion. These types of examples show where the DTW code breaks down. The code cannot decipher whether a proxy value is from the beginning or the end of the excursion, and the code is unlikely to create such large gaps in the record. The code either aligns all of the points to before or after the excursion. For these types of examples, additional biostratigraphic data would be valuable to constrain some of the data points and differentiate between Paleocene and Eocene-deposited sediment; these additional data would show the significant amount of time between the data points in the preserved record.

4.5 Discussion

For most alignments of fluvial-deltaic records with a given target and candidate record, DTW will create the best alignment when cross-correlation and overlap are maximized. This usually occurs when g=1; edge can vary significantly. For the candidate records, there is a large difference in whether the start and end points of the candidate record occur at many different times in comparison with the start and end points of the target record. There is less variation in the changes in relative sedimentation rates seen in the candidate record in comparison with the
target record. For a candidate record with no evidence of the PETM excursion, the alignment to
the target record becomes much less reliable because DTW has less information from which to
align. For these kinds of examples, additional biostratigraphic data are needed to constrain the
alignments. DTW proved effective in aligning proxy records that were very poorly preserved, as
long as the record had some preservation of the PETM excursion. For most of the TURBO2
alignments, changing $g$ and edge does not significantly change the MAE. This is mostly a result
of the differences between the TURBO2 model and the Trampush & Hajek (2017) stochastic
sedimentation model. There is no noise added to the TURBO2 record whereas the input record in
the Trampush & Hajek (2017) has added noise. The shape of the records output from TURBO2
provide enough constraints on which the TURBO2 model can easily align back to the input
record.

4.6 Conclusion

The results of this chapter show that bioturbation and dissolution usually decrease the
accuracy of the alignment. Dissolution may only have an appreciable effect on the accuracy of
the alignment if there was sufficient dissolution to create a clay layer (Fig. 12). In fluvial-deltaic
records, DTW will be relatively accurate if the candidate record shows evidence of large-scale
features in the target record (for instance the PETM excursion).

Comparison of the output of DTW performed on the deep-sea sediment model output
compared to output records from the fluvial-deltaic model yields insight into how DTW can be
used effectively in the two different scenarios. In most alignments, the most accurate alignment
will be found simply by finding the maximum cross-correlation and overlap generated from
testing a range of $g$ and edge values. In fluvial-deltaic records from the Trampush & Hajek
(2017) model, if the record is too poorly preserved, maximizing cross-correlation and overlap
will not generate the most accurate alignment. DTW becomes inaccurate for aligning a candidate record to a target record when all of the proxy values of a candidate record could be aligned to the beginning of the target record, to the end of a target record, or a portion of values could be aligned to the beginning of the record and a portion of values could be aligned to the end of the record (e.g. Fig. 10). For the records from the fluvial-deltaic model, the best alignments usually have a $g=1$; the warping path is not constrained. For the records from the deep-sea model, $g$ and $edge$ does not significantly change the alignment. The deep-sea model results are not significantly affected by $g$ and $edge$ because PETM deep-sea records were deposited more continuously than in fluvial-deltaic records, as reflected in the Trampush & Hajek (2017) and TURBO2 models (Westerhold et al., 2008). Different types of deposition in fluvial-deltaic environments lead to more dynamic sedimentation (Bowen et al., 2015; Westerhold et al., 2018). This difference causes the deep-sea records to have more accurate alignments, with a large possible range of $g$ and $edge$.

The application of DTW is somewhat different when using observed data. For a model, a target record is an idealized, complete record. However, for real, observed data we cannot have a record that is totally complete and undistorted. When we align a candidate record to a target record, even the most accurate alignment may not yield enough information into how the candidate record would align to the original paleoceanographic signal. Additionally, for the records from the TURBO2 model, there was no noise added to the model that simulates the local effects (such as changing coccolith assemblages) that creates more difficulty in DTW alignments. This chapter showed insight into how the accuracy of DTW alignments can be maximized in different types of records, but significant errors will still remain when using DTW.
References


Figure 1: Range of cross-correlation, overlap, and MAE values (in yr) obtained from varying g and edge parameters. In this example, g ranged from 0.1 to 2 and edge ranged from 0.1 to 2. A. Model 1 run with a minimum MAE of 10,500 yr (in red). B. Model 2 run with a minimum MAE of 19,000 yr (in red). C. Model 3 run with a minimum MAE of 18,300 yr (in red). D. Model 4 run with a minimum MAE of 20,200 yr.
Figure 2: Fully preserved PETM proxy record (in time) over 350kyr that will be used as the target record in DTW. Obtained with permission from Trampush & Hajek (2017).
Figure 3: A. Truncated double-Pareto distribution of sedimentation rates with High Sed Rate/Low Variability and Low Sed Rate/High Variability model. For each year for 350 kyr the proxy value will be preserved if the annual sedimentation is positive, eroded if the annual sedimentation is negative, or there will be non-deposition if the annual sedimentation is 0. Obtained from Trampush & Hajek (2017) B. Figure depicts which sections of the 350 kyr are preserved (in color) based on the sedimentation distribution from a High Sed Rate/Low Variability model. Obtained with permission from Trampush & Hajek (2017).
Figure 4: Example output records from the Trampush & Hajek (2017) model from each of the four different depositional settings. Obtained with permission from Trampush & Hajek (2017).
Figure 5: In red is a synthetic bulk carbonate PETM $\delta^{13}$C record in time. Various profiles of CaCO$_3$ abundance in gray scale. Starting with high dissolution/slow recovery in black, then high dissolution/moderate recovery, high dissolution/fast recovery, moderate dissolution, and then low dissolution in the lightest gray color.
Figure 6: TURBO2 results in depth of varying mixed layer depths and abundance profiles applied to the synthetic PETM δ¹³C profile. Input record in black, and TURBO2 output in red. The output record (in red) will be aligned back to the input record (in black) using DTW. Clay layer in gray. From top to bottom row: bioturbation low, moderate, high. From left to right: low dissolution, moderate dissolution, high dissolution/fast recovery, high dissolution/moderate recovery, high dissolution slow recovery (same figure as in Chapter 3, Figure 4)
Figure 7: An alignment of one output record from each model to the input signal. The mean absolute error (MAE) in each alignment is near the median MAE (in yr) for a given model; it represents an alignment with the average accuracy for the model. A. Model 1 run with a MAE of 10,500 yr. B. Model 2 run with an MAE of 19,000 yr. C. Model 3 run with an MAE of 18,300 yr. D. Model 4 run with an MAE of 20,200 yr.
Figure 8: Distribution of $g$ and $edge$ values in each of the alignments of Trampush & Hajek (2017) records that minimized the mean absolute error (MAE).
Figure 9: Mean absolute error (MAE) (in yr) distribution for each of the four models. A. Model 1 B. Model 2. C. Model 3. D. Model 4.
Figure 10: Alignments with a mean absolute error (MAE) greater than 80,000 yr. A. Model 3 MAE of 185,000 yr B. Model 4 MAE 163,000 yr. C. Model 4 MAE 113,000 yr.
Figure 11: Distribution of $g$ and $edge$ values in one of the alignments of TURBO2 records. Mean absolute error (MAE) (in cm).
Figure 12: Mean absolute error (MAE) of each of the alignments of the TURBO2 outputs to the input record.
Chapter 5

Expanding the capabilities of Dynamic Time warping to employ a multivariate approach

Abstract

Researchers have attempted to understand which Paleocene Eocene Thermal Maximum (PETM) records are the most affected by carbonate dissolution; they also have attempted to correlate multiple $\delta^{13}C$ records at different sites. X-ray fluorescence (XRF) core scanners determine the chemical compositions of Ba & Fe in sediments, and can resolve precessional cycles preserved in the proxy record. The precessional cycles of multiple proxy records were aligned using dynamic time warping (DTW). DTW has been used as a tool to align geochemical proxy records at different locations. In previous work, DTW has been used to align one type of proxy (such as $\delta^{13}C$) at one location to the same type of proxy at another location; this approach is defined as a univariate alignment. The capabilities of DTW can be expanded, however, to employ a multivariate approach, where multiple proxies at one location can be aligned to multiple proxies at another location. Here we aligned both Ba & Fe proxies from Maud Rise & Walvis Ridge simultaneously as a case example of a multivariate alignment. Combining the alignment of Ba & Fe into a multivariate alignment for both Site 690 & Site 1262 aligned to Site 1263, created alignments that were similar to those generated using standard cyclostratigraphic approaches.

5.1 Introduction

Geochemical proxies are inorganic or organic material preserved in sediment that store geochemical information of past climates and environments (e.g., Henderson, 2002). These proxies contain information about paleotemperature, ocean circulation, ocean productivity, pH,
atmospheric CO$_2$ and more (e.g., Emiliani, 1955; Epstein et al., 1951; Hemming & Hanson, 1992; Henderson, 2002; Higginson, 2009; Sarmiento & Toggweiler, 1984; Spivack et al., 1993; Urey et al., 1951). The most commonly used geochemical proxies are preserved in carbonate fossils (e.g., Henderson, 2002). These fossils are formed from zooplankton, such as foraminifera, or from phytoplankton, such as coccolithophorids (e.g., Wefer et al., 1999). The most commonly used proxy derived from carbonate material is $\delta^{13}C$. $\delta^{13}C$ is a ratio of the $^{13}C$ isotope to the $^{12}C$ isotope (e.g., Kendall & Caldwell, 1998).

$$
\delta^{13}C = \left( \frac{^{13}C}{^{12}C} \right)_{sample} - \left( \frac{^{13}C}{^{12}C} \right)_{standard} \right) \times 1000 \%o
$$

During the Paleocene-Eocene Thermal Maximum (PETM), there was an injection of CO$_2$ with low $\delta^{13}C$ carbon values that drove a negative shift in the $\delta^{13}C$ of the ocean as recorded in foraminifera, coccolithophorids, and other carbonate material (Kennett & Stott, 1991; McInerney & Wing, 2011). This isotopically “light” carbon injection into the ocean also lowered the pH and carbonate ion content of the seawater causing a shoaling of the lysocline and calcite compensation depth (CCD) which resulted in dissolution of sea-floor carbonate. The dissolution of sea-floor carbonate caused much of the proxy information to be erased at the onset of the event in deep-sea sites (e.g., Kelly et al., 2010; Bralower et al., 2014; Zachos et al., 2005; Ridgwell, 2007). In order to understand how to reconstruct the PETM, researchers have attempted to identify which sites are the most affected by carbonate dissolution; they also have attempted to correlate multiple $\delta^{13}C$ records at different sites to yield enough information to reconstruct the PETM.
There are, however, other geochemical proxy records that yield information about the PETM, such as Ca, Fe, and Ba. Röhl et al. (2007) investigated the abundance of Ca, Fe, and Ba, in various marine sections. These records, when obtained with X-ray fluorescence core scanners, often have a better signal-to-noise ratio than other physical property measurements, and can analyze sediments at sub-millimetric intervals (Jones et al., 2013; Croudace & Rothwell, 2015; Richter et al., 2006; Tjallingii et al., 2007). The primary Ca signal in sediment is driven by the CaCO$_3$ wt. %, which decreases drastically as the lysocline and CCD shoals, and sea-floor carbonate undergoes dissolution. The primary Fe signal serves almost as an inverse of CaCO$_3$. When the carbonate content is high, Fe is low. There is a low signal to noise ratio of Ca when carbonate is high (Röhl et al., 2007). Some contend that the Ba signal is driven by export paleoproduction (Bains et al., 2000; McManus et al., 1998; Paytan et al., 1993). Dickens et al. (2003) contends that the Ba signal is driven largely by the supply of Ba to the ocean either from rivers or methane hydrates. Ba, overall, has a higher signal to noise ratio than Ca and Fe (Röhl et al., 2007). During the PETM, all three of these elemental proxy records change drastically. There is a negative excursion in Ca, and positive excursions in Ba & Fe at the onset of the PETM, with the onset and recovery coinciding with the CaCO$_3$ dissolution and recovery during the PETM. One of the advantages of using Ba and Fe records, is that during intervals of high CaCO$_3$ dissolution (intervals where $\delta^{13}$C would not be preserved), their abundances do not decrease to 0 as does Ca.

In all three of these types of records, the precision at which they can be measured allows for measurement of astronomical signals called Milankovitch cycles. As the Earth orbits around the Sun, it interacts with other planets, the Sun, and the moon, creating cyclostratigraphic frequencies in geochemical proxy records (Hinnov & Ogg, 2007). Eccentricity, the shape of the
Earth’s orbit, can be seen in 100 kyr and 400 kyr cycles in sediment. Obliquity, the Earth’s tilt, is observed in 41 kyr cycles. Precession is the Earth’s “wobble” results in ~20 kyr cycles (Hinnov & Ogg, 2017). Each of these cycles can be preserved in geochemical proxy records, and allow for geochemical proxy records to be correlated with one another and with relative time. Precessional cycles (~20 kyr) provide the shortest frequency bands with which proxy records can be correlated. In the PETM δ¹³C signals, the CIE dominates the records, and the precessional cycles are too low-resolution to be correlated. However, in Röhl et al. (2007), precessional cycles for XRF core scanning records of Ba & Fe were correlated to each other. The precessional cycles in one of the proxy records can disappear due to smearing of the record, such as in Site 1263 Fe, so both proxy records are needed to accurately count the number of precessional cycles in the record. The precessional cycles from these records were aligned to each other manually.

In our study, the precessional cycles and the PETM excursion of multiple proxy records were aligned using dynamic time warping (DTW). DTW has been used as a tool to geochemical proxy records at different locations. In previous work, DTW has been used to align one type of proxy (such as δ¹³C) at one location to the same type of proxy at another location (e.g., Ajayi et al., 2020; Chapter 2); this approach is defined as a univariate alignment. The capabilities of DTW can be expanded, however, to employ a multivariate approach, where multiple proxies at one location can be aligned to multiple proxies at another location. Previously, we aligned δ¹³C proxies from Maud Rise & Walvis Ridge (Ajayi et al., 2020; Chapter 2). In this chapter, we aligned both Ba & Fe proxies from Maud Rise & Walvis Ridge simultaneously. One of the drawbacks of using a univariate DTW approach on observed data is that the alignment depends on how well the target record is preserved in sediment. For instance, in Chapters 2 and 3, Site 1263 is the target record. In this case, the alignments of the candidate record to the target record
depends on the assumption that the temporary reversal of slope in Site 1263 is a global signal that is not preserved in most other sites. If this assumption is not correct, and this feature is simply an artifact of changing coccolith assemblages or some other local effect (e.g., Bralower, 2002; Stoll, 2005), the alignments of the candidate records are less useful. In order for a target record to be useful, its preserved signal must reflect a complete paleoenvironmental signal. Unfortunately, no record completely preserves the same signal, with different local effects (such as bioturbation, dissolution, winnowing, and changing nannofossil assemblages) that change the proxy record at one location. If one of these factors cause a global paleoenvironmental signal to be less completely preserved in sediment, the target record is less useful. In addition, the candidate record at a particular location might be useful for one proxy record than the other. For instance, in Site 690 there is significant smearing of the record from 167 mbsf to 169 mbsf (Fig. 3), where the Milankovitch cycles can’t be clearly identified. By aligning multiple proxy records simultaneously, local effects that affect only one proxy record, would be less likely to affect the entire alignment.

5.2 Methods

We investigated a method to expand the capabilities of the univariate DTW code we have previously used (Hay et al., 2019) by adding a multivariate approach. Fig. 1A & Fig. 1B have two different warping paths, indicating two different univariate alignments of Site 690 to Site 1263 of two different proxy records. A multivariate approach aligns two different proxy records at once at two different sites (Fig. 2). In this approach, the same warping path is drawn to align the depth axis of Site 690 to the depth axis of Site 1263 for the two different proxy records. The cumulative squared difference map in Fig. 2 is determined by averaging the cumulative squared difference maps created in the alignment of Site 690 Ba to Site 1263 Ba and Site 690 Fe to Site
1263 Fe (Fig. 1A & Fig. 1B). For a multivariate alignment, \( g \) and edge values are selected that create one given warping path (Fig 2A & Fig. 2B), with two different cross-correlation and overlap values (one for the Ba alignment and one for the Fe alignment). \( G \) and edge values therefore must be selected to create a warping path that maximizes cross-correlation and overlap both for the Ba & Fe alignments. In order to improve the resolution of the precessional cycles, a Gaussian filter was applied to each of these records to filter out noise using Acycle (Li et al., 2019). The common logarithm was taken for the Site 1263 Fe, Site 1263 Ba, and Site 1262 Fe records to improve the signal-to-noise ratio between the PETM excursion and precessional cycles. The peak of the PETM excursion was also cut-off for the Site 690 Ba, Site 1263 Fe, and Site 1262 Fe records to improve the signal-to-noise ratio between the PETM excursion and precessional cycles. The Fe & Ba records after processing the records are shown in Fig. 3. Each of the alignments performed are shown in Table 1.

<table>
<thead>
<tr>
<th>Sites Aligned</th>
<th>Type of Alignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Site 690 to Site 1263</td>
<td>Ba univariate</td>
</tr>
<tr>
<td>Site 690 to Site 1263</td>
<td>Fe univariate</td>
</tr>
<tr>
<td>Site 1262 to Site 1263</td>
<td>Ba univariate</td>
</tr>
<tr>
<td>Site 1262 to Site 1263</td>
<td>Fe univariate</td>
</tr>
<tr>
<td>Site 690 to Site 1263</td>
<td>Multivariate (Ba &amp; Fe aligned simultaneously)</td>
</tr>
<tr>
<td>Site 1262 to Site 1263</td>
<td>Multivariate (Ba &amp; Fe aligned simultaneously)</td>
</tr>
</tbody>
</table>

Table 1: Sites and proxy records to align

5.3 Results

Figs. 4 & 5 show the alignments of Site 690 to Site 1263 and Site 1262 to Site 1263 for both the Ba & Fe count. In each panel, the results are shown for both the univariate and multivariate alignment. The Ba & Fe counts were aligned simultaneously for the multivariate alignments and the Ba & Fe were aligned separately for the univariate alignments. The multivariate and univariate alignments for Site 1262 to Site 1263 (Fig. 4) show very small
differences. The multivariate and univariate results for the alignment of Site 690 to Site 1263 (Fig. 5) show larger differences. In Fig. 4A, the multivariate alignment of Ba has a longer positive Ba PETM excursion, with an earlier onset and later recovery, than the univariate alignment. In Fig. 5B the multivariate alignment shows Ba reaching the peak of the excursion earlier than the univariate alignment. Each of the alignments in Fig. 4 & Fig. 5 shifted the depth axis of either Site 690 or Site 1262 to align with Site 1263.

Fig. 6 shows how bulk carbonate δ¹³C values would align for each of these alignments as a consequence of the depth shifts of Site 690 & Site 1262 created by the Ba & Fe alignments to Site 1263. For each of these alignments, the Site 690 & Site 1262 δ¹³C records have a delayed onset, occurring after the Site 1263 δ¹³C onset. The univariate alignment of Site 1262 Fe to Site 1263 Fe results in the latest onset, with a very condensed record overall. The univariate alignment of Site 690 Fe to Site 1263 Fe has an expanded PETM interval, with a very late recovery, and a long period of intermediate values in the middle of the excursion. Overall, the multivariate alignments of Site 690 to Site 1263 and Site 1262 to Site 1263 more closely align to the shape of Site 1263, with a lagged onset of the PETM excursion.

Röhl et al. (2007) performed the same alignments of Site 690 to Site 1263 and Site 1262 to Site 1263 by manually identifying and aligning precessional cycles in Ba and Fe. Discrete data points at precessional scale intervals (~20 kyr) aligned individual depths of Site 690, Site 1262, and Site 1263. These discrete data points are called ‘tie points.’ At each Röhl et al. (2007) tie point, we found the mean absolute error (MAE) with the same data point in our alignment.

\[
\text{Mean Absolute Error} = \frac{\sum_{i=1}^{n} |\text{DTW alignment depth} - \text{Rohl tie point depth}|}{\text{total number of values}}
\]
An example of a MAE calculation is shown in Table 2.

Table 2: example MAE calculation of a Röhl et al. (2007) alignment with the DTW alignment

<table>
<thead>
<tr>
<th>Site 1262 original depth</th>
<th>Röhl et al. (2007) alignment depth</th>
<th>DTW alignment depth</th>
</tr>
</thead>
<tbody>
<tr>
<td>135 m</td>
<td>330 m</td>
<td>332 m</td>
</tr>
<tr>
<td>137 m</td>
<td>332 m</td>
<td>333 m</td>
</tr>
<tr>
<td>140 m</td>
<td>335 m</td>
<td>336 m</td>
</tr>
</tbody>
</table>

Mean Absolute Error $\frac{|332−330|+|333−332|+|336−335|}{3} = 1.33$ m

Table 3 shows the MAE for each of the alignments. The MAE corresponds to the mean distance between the Röhl et al. (2007) tie point and the DTW alignment value for a given alignment. For all of the alignments, the multivariate approach is more similar to the Röhl et al. (2007) alignment. The multivariate approach improves the alignment of Site 690 to Site 1263 by a larger factor than the alignment of Site 1262 to Site 1263. Figs. 7-10 show the comparison of Röhl et al. (2007) tie points with the DTW alignments. The lines drawn on the figure from the Röhl et al. (2007) tie point to either Site 690 or Site 1262 show the distance between Röhl et al. (2007) tie point and the DTW alignment for each tie point.

Table 3: MAE between Röhl et al. (2007) alignment and DTW alignment

<table>
<thead>
<tr>
<th></th>
<th>MAE (m) with Röhl (2007)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Site 690 to Site 1263 Ba univariate</td>
<td>0.596</td>
</tr>
<tr>
<td>Site 690 to Site 1263 Fe univariate</td>
<td>0.786</td>
</tr>
<tr>
<td>Site 1262 to Site 1263 Ba univariate</td>
<td>0.450</td>
</tr>
<tr>
<td>Site 1262 to Site 1263 Fe univariate</td>
<td>0.381</td>
</tr>
<tr>
<td>Site 690 to Site 1263 Multivariate (Ba &amp; Fe aligned simultaneously)</td>
<td>0.304</td>
</tr>
<tr>
<td>Site 1262 to Site 1263 Multivariate (Ba &amp; Fe aligned simultaneously)</td>
<td>0.278</td>
</tr>
</tbody>
</table>
5.4 Discussion

All of our alignments show that aligning cyclostratigraphic cycles of Fe & Ba cause the δ\textsubscript{13}C onset to be lagged in Site 1262 & Site 690 in comparison to Site 1263 (Fig. 6). In Ajayi et al. (2020) and Zachos et al. (2005), these onsets were synchronous. Manual alignment of precessional cycles by Röhl et al. (2007), however, also results in a delayed δ\textsubscript{13}C onset in both Site 690 & Site 1262 when Ba & Fe are aligned.

Our results, however, show that precessional cycles can be aligned automatically using a multivariate approach, and create improved results over a univariate approach. In a univariate alignment, such as in the alignment of Site 690 Fe to Site 1263 Fe, the disappearance of the cyclicity in Fe during the recovery phase of the PETM created an alignment significantly different than the Röhl et al. (2007) alignment, indicated by a MAE of 0.786 m. The alignment of Site 690 Ba to Site 1263 Ba yielded a closer alignment, with a MAE of 0.596 m. However, combining the alignment of both Ba & Fe into a multivariate approach yielded the closest alignment to the Röhl et al. (2007) alignment with a MAE of 0.304 m. Figs. 7-10 do not show any systematic error between our alignment and Röhl et al. (2007) tie points, any errors occurred randomly at different parts of the record.

5.5 Conclusion

Our results show that multivariate alignments have the potential to improve the accuracy of DTW alignments. This study, to our knowledge, is the first to use a multivariate DTW approach in a geosciences application. For both the alignments of Site 690 & Site 1262 to Site 1263, combining the alignment of Ba & Fe into a multivariate alignment created alignments that were closer to Röhl et al. (2007) alignments, and created δ\textsubscript{13}C plots that were more plausible. For
both Ba & Fe, there were intervals in both of the records where one of the variables were unreliable and smeared out, so combining into multivariate approach removes the impact of one of the records to distort the whole alignment.

The multivariate alignments performed here are a case study illustrating the potential of multivariate alignments. For these alignments of Ba & Fe, there is significant uncertainty in both identifying and aligning the precessional cycles correctly. One would expect that the alignments of $\delta^{13}$C (Fig. 6) would illustrate synchronous carbon isotope excursions, but that is not the case. This result could be indication that the precessional cycles were not correctly aligned in this study.

In future work, additional proxy records can be aligned at once, to see if the alignments will improve even further. Milankovitch cycles are not always clearly detected throughout a record. The more proxy records are used, the more likely we can accurately align these cycles. We could add the Ca proxy, to the Ba & Fe proxy alignment to see if aligning precessional cycles on additional variables would improve the alignment. We could also align $\delta^{13}$C simultaneously with Ba & Fe, to see if an alignment can be created where the PETM onset of all three proxy records occur at the same time. For the $\delta^{13}$C record, DTW is mostly aligning the PETM CIE. For the Ba & Fe records, DTW is aligning both the CIE and the precessional cycles. Particularly in the PETM, during the recovery period, there is significant uncertainty in the $\delta^{13}$C record, carbon isotope values become nearly constant. In this interval, the alignment of precessional cycles of Ba & Fe records.

In other datasets, precessional cycles from other proxies, such as $\delta^{18}$O records could be aligned in future work on longer time scales. Multivariate DTW could help refine longer age models by increasing the accuracy of orbital chronology.
References


Figures

Figure 1: Warping paths for two different univariate DTW alignments. In the left panel is the univariate alignment of Site 690 Ba to Site 1263 Ba. In the right panel is the univariate alignment of Site 690 Fe to Site 1263 Fe.
Figure 2: Warping path for one multivariate DTW alignment of two different proxies. In the left panel is the multivariate alignment of Site 690 Ba to Site 1263 Ba. In the right panel is the multivariate alignment of Site 690 Fe to Site 1263 Fe.
Figure 3: Site 690, Site 1262, and Site 1263 Ba & Fe XRF core-scanning records used in alignment (obtained from Röhl et al. (2007))
Figure 4: Multivariate and univariate alignments of Site 1262 to Site 1263 for Ba & Fe.
Figure 5: Multivariate and univariate alignments of Site 690 to Site 1263 for Ba & Fe.
Figure 6: $\delta^{13}$C alignments created by the Ba & Fe alignments of Site 690 and Site 1262 to Site 1263
Figure 7: Univariate alignments of Site 690 to Site 1263 for Ba & Fe
Figure 8: Univariate alignments of Site 1262 to Site 1263 for Ba & Fe
Figure 9: Multivariate alignments of Site 690 to Site 1263 for Ba & Fe
Figure 10: Multivariate alignments of Site 1262 to Site 1263 for Ba & Fe
Chapter 6

Conclusions

6.1 Summary

In this dissertation, we developed DTW as a tool to align chemostratigraphic records from the PETM. Alignments of chemostratigraphic records were previously done subjectively, while our study uses a statistical approach. By aligning chemostratigraphic records during the PETM, we can better understand the effects of carbon input to the ocean and atmosphere. DTW was shown to reliably align PETM geochemical proxy records from a variety of depositional settings. We also gained new insights into the fidelity of proxy records from the PETM.

6.2 Key Contributions

Chapter 2:

We found that aligning proxy records using DTW yielded new insights into the relative completeness of two classic PETM records from Walvis Ridge in the South Atlantic Ocean and Maud Rise in the Southern Ocean. The alignment of Site 690 to Site 1263 identifies a gap in Site 690, indicating that the Site 690 bulk carbonate record may not have preserved the minimum excursion value. Dissolution may have impacted Site 690 to a greater degree than previously thought (Bralower et al., 2014a). Alternatively, Site 690 may simply have experienced a lower magnitude CIE. We also found that DTW was largely able to reproduce the correlations established by expert, but non-automated and more subjective means.

Chapter 3:

We used a bioturbation model to evaluate how bioturbation and dissolution affects the preservation of synthetic PETM bulk carbonate $\delta^{13}$C signals under a variety of scenarios of seafloor dissolution and mixed layer depths. The model results show that increasing bioturbation
slightly decreases the magnitude of the CIE and lengthens the perceived duration of the onset. Dissolution does not begin to have a noticeable effect on the shape and magnitude of the CIE until a clay layer starts to develop, at which time gaps are created in the δ₁³C record. Additionally, the temporary reversal in slope in bulk carbonate δ₁³C records at Site 1263 and Site 690 is preserved when there are low amounts of bioturbation and relatively lower amounts of dissolution (if a clay layer develops, it must be relatively small). These results would support the hypothesis that there were multiple injections of light carbon during the PETM, the effects of which are only preserved in some δ₁³C records.

Chapter 4:

A deep-marine and fluvial-deltaic model were used to create a synthetic preserved proxy record under a variety of depositional settings from a PETM paleoenvironmental signal. Dynamic time warping (DTW) is used to align the model output records (preserved proxy records) to the model input record (complete paleoenvironmental signal). For the records from the fluvial-deltaic model, the best alignments usually have a g=1. For the records from the deep-sea model, g and edge do not significantly change the alignment. Bioturbation and dissolution usually decrease the accuracy of the alignment. Dissolution may only have an appreciable effect on the accuracy of the alignment if there was sufficient dissolution to create a clay layer. In fluvial-deltaic records, DTW was relatively accurate if the candidate record shows evidence of large-scale features in the target record (for instance the PETM excursion).

Chapter 5:

In previous work, DTW has been used to align one type of proxy (such as δ₁³C) at one location to the same type of proxy at another location; this approach is defined as a univariate alignment. The capabilities of DTW can be expanded, however, to employ a multivariate
approach, where multiple proxies at one location can be aligned to multiple proxies at another location; we aligned both Ba & Fe proxies from Maud Rise & Walvis Ridge simultaneously. For both Site 690 & Site 1262 aligned to Site 1263, combining the alignment of Ba & Fe into a multivariate alignment, created alignments that were more similar to Röhl et al. (2007) alignments. This case example of a multivariate approach was the first application of multivariate DTW alignment to geosciences.

6.3 Future Research Directions

We learned new insights into the fidelity of well-established PETM carbon isotope records. In Chapter 3, we posited that the temporary reversal in slope in Site 690 & Site 1263 corresponded to multiple injections of light carbon during the PETM. We can further investigate this hypothesis by expanding the capabilities of both TURBO2 and DTW. We can modify TURBO2 to model bioturbation and dissolution on bulk records with changing species assemblages, to see if the temporary reversal in slope can be reproduced under these conditions. We can also expand the multivariate DTW approach, to align δ\textsubscript{13}C simultaneously with Ba & Fe, to see if the temporary reversal in slope in Site 690 & Site 1263 are synchronous. If they are not synchronous, the temporary reversal in slope most likely is site-specific, and does not correspond to a global signal.

DTW can also be expanded to be used in many different applications. The multivariate approach can be used to simultaneously align even more proxies at once. In addition, precessional cycles can be aligned from other proxy records such as the δ\textsubscript{18}O proxy. Long-term benthic δ\textsubscript{18}O could be aligned, to help refine age models.

The results of DTW can be strengthened and weakened by developing a more robust measurement of uncertainty in each alignment. Uncertainty was examined briefly in the
Supplementary Material section (Figs. S2-S6). The degree of uncertainty in each alignment will strongly impact the degree of advantage DTW yields over more subjective methods of alignments.
Appendix

Chapter 2 Supplementary Material

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Section 1: Range of Possible Alignments with varying g and edge parameters
Section 2: Statistical significance of alignments
Section 3: Creating age models for Site 690, Site 1262, and Site 1265
Section 4: Site 690 bulk record
Section 5: Sample DTW alignment of a target and candidate record
Introduction

The supplemental information section is a selection of five sections that show figures and text that support the methods and discussion point in the paper “Dynamic Time Warping as a means for aligning chemostratigraphic records of the Paleocene-Eocene Thermal Maximum.”

Section 1: Range of Possible Alignments with varying g and edge parameters

For the δ¹³C alignments of Site 1262, Site 1265, and Site 690 to Site 1263, a range of g and edge parameters are investigated, to show how it affects the alignment.

As stated in the Methods section, “Two “penalty” factors can be applied to the difference matrix ‘d’: the edge parameter (edge) and the diagonal parameter (g). Edge reflects the presumed extent to which the two data series span the same epoch, and g controls the amount of allowable change in relative sedimentation rates. After considerable experimentation with various g and edge parameter values (Supplemental Information Section 1) we set the g and edge parameters equal to the default values of 1; i.e., we did not apply penalties. Alignments with alternate g and edge parameter values are shown in the Supplemental Information Section 1.”

A value of g>1 increases the likelihood that the candidate record and the target record are assigned the same relative sedimentation rate (there are no gaps assigned to the candidate record and the warping path is linear and diagonal). A value of g<1 decreases the likelihood that the candidate record and the target record have the same relative sedimentation rate (there are more likely large gaps in the candidate record or intervals of compression, and the warping path deviates from linear). A value of edge>1 increases the likelihood that the start point and end point of the candidate record and the target record occur at the same time. A value of edge<1 increase the likelihood that the start point and end point of the candidate record and the target record occur at different times.

Figures S1, S3, and S5 show the cross-correlation and overlap value obtained for the alignment of the candidate record to the target record. Each blue stem on the figures correspond to one DTW run where a certain g and edge were chosen. g is displayed on the x axis, and edge is displayed on the y axis. g values investigated ranged from 0.6, 0.7, …, 1.3 and edge values ranged from 0.1, 0.2, …, 2. The left panel on each figure shows the resulting cross-correlation on the z-axis for each DTW run and the right panel shows the resulting overlap on the z-axis. The best alignments are produced by maximizing both the cross-correlation and overlap for a given g and edge run. The stem shaded red in each of these plots corresponds to the cross-correlation and overlap when g=1 and edge=1. In each of these plots, g=1 and edge=1 maximizes cross-correlation and overlap if maximizing cross-correlation is slightly favored over maximizing overlap. In order to look at the range of possible alignments based on varying the g and edge parameter, we selected two different runs with different g and edge settings that also relatively maximized cross-correlation and overlap. Figures S2, S4, and S6 show how candidate
record would align to the target record based on the g and edge parameter chosen. The red lines show the range of possible placements of each data point of the candidate record.

Figure S2 shows that for the alignment of Site 1262 to Site 1263 varying the g and edge parameters changes the alignment before the onset, during the recovery, after the recovery phase of the CIE. During most of the CIE, however, the alignment does not change. Figure S4 shows that the alignment of Site 1265 to Site 1263 only changes slightly before the onset after the recovery phase of the CIE. Figure S6 shows the alignment of Site 690 to Site 1263 shows that varying the g and edge parameters changes the alignment after the recovery of the CIE. It also changes the alignment during the CIE, meaning there is some uncertainty at a crucial part of the alignment.
Figure S1: 3-D stem plot of alignment of Site 1262 $\delta^{13}$C to Site 1263 $\delta^{13}$C. Each stem on the figure corresponds to one DTW run with an inputted $g$ and edge parameter. $g<1$ is not displayed on this figure because the resulting overlap was so low that it produced an error in the code. $g=1$ and edge=1 is displayed in red, and represents the alignment that maximizes cross-correlation and overlap.
Figure S2: alignment of Site 1262 $\delta^{13}$C to Site 1263 $\delta^{13}$C. This figure shows how different g and edge values chosen from Fig. S1 affect the alignment. The blue line is the target record, Site 1263. The black line with the squares representing the specific data points correspond to a g=1 and edge=1. The other two gray lines correspond to alternate g and edge values that yield good alignments. The red lines correspond to the range of results obtained from varying the g and edge parameters.
Figure S3: 3-D stem plot of alignment of Site 1265 $\delta^{13}C$ to Site 1263 $\delta^{13}C$. Each stem on the figure corresponds to one DTW run with an inputted g and edge parameter. g=1 and edge=1 is displayed in red, and represents the alignment that maximizes cross-correlation and overlap.
Figure S4: alignment of Site 1265 $\delta^{13}$C to Site 1263 $\delta^{13}$C. This figure shows how different g and edge values chosen from Fig. S3 affect the alignment. The blue line is the target record, Site 1263. The black line with the squares representing the specific data points correspond to a g=1 and edge=1. The other two gray lines correspond to alternate g and edge values that yield good alignments. The red lines correspond to the range of results obtained from varying the g and edge parameters.
Figure S5: 3-D stem plot of alignment of Site 690 $\delta^{13}$C to Site 1263 $\delta^{13}$C. Each stem on the figure corresponds to one DTW run with an inputted $g$ and edge parameter. $g=1$ and edge=1 is displayed in red, and represents the alignment that maximizes cross-correlation and overlap.
Figure S6A: alignment of Site 690 $\delta^{13}$C to Site 1263 $\delta^{13}$C. This figures shows how different g and edge values chosen from Fig. S5 affect the alignment. The blue line is the target record, Site 1263. The black line with the squares representing the specific data points correspond to a g=1 and edge=1. The other two gray lines correspond to alternate g and edge values that yield good alignments. The red lines correspond to the range of results obtained from varying the g and edge parameters. This alignment shows uncertainty throughout the CIE.
Figure S6B: alignment of Site 690 $\delta^{13}$C to Site 1263 $\delta^{13}$C. This figures shows how adding noise to the Site 690 record changes uncertainty in the alignment. different g and edge values chosen from Fig. S5 affect the alignment. The blue line is the target record, Site 1263. The black line with the squares representing the specific data points corresponding to no noise added. The red lines correspond to the range of results obtained from varying the amount of noise in the Site 690 record. This alignment shows uncertainty throughout the CIE.
Section 2: Statistical significance of alignments

As stated in the Methods section of the main text:

“The statistical significance of these Walvis Ridge transect and Site 690 alignments was evaluated by assessing the distribution of cross-correlation values produced by alignments of synthetic (random) candidate records (Site 1262, Site 1265, and Site 690) to the Site 1263 target record. One hundred thousand synthetic random-walk sequences were created using a Monte Carlo method (Haam & Huybers, 2010; Hay et al., 2019). Each of these synthetic sequences had the same number of data points as the candidate records. Each sequence was aligned to Site 1263 yielding a distribution of 100,000 cross-correlation values. The cross-correlation of the alignment of the actual candidate record to Site 1263 was compared to this distribution. The p-value is the proportion of cross-correlation values that are equal or higher in the distribution of alignments of synthetic sequences to Site 1263.”

Figures S7, S8, and S9 show a histogram of cross-correlation values obtained from 100,000 alignments of the candidate record to Site 1263. The x-axis shows the range of cross-correlation values being evaluated, and the y-axis shows the number of alignments that yielded cross-correlation values in that range. The cross-correlation value for the alignment of Site 690 to Site 1263 was 0.974, yielding a p-value of 0.004. The cross-correlation value for the alignment of Site 1262 to Site 1263 was 0.957, yielding a p-value of 0.057. The cross-correlation value for the alignment of Site 1265 to Site 1263 was 0.989, which is a greater value than all of the 100,000 synthetic runs, thus yielding a p-value of 0.000.
Figure S7: Distribution of cross-correlation values for 100,000 synthetic $\delta^{13}$C records to assess the statistical significance of the alignment of Site 690 to Site 1263. The cross-correlation value for the alignment of Site 690 to Site 1263 was 0.974, yielding a p-value of 0.004.
Figure S8: Distribution of cross-correlation values for 100,000 synthetic δ¹³C records to assess the statistical significance of the alignment of Site 1262 to Site 1263. The cross-correlation value for the alignment of Site 1262 to Site 1263 was 0.957, yielding a p-value of 0.057.
Figure S9: Distribution of cross-correlation values for 100,000 synthetic δ^{13}C records to assess the statistical significance of the alignment of Site 1265 to Site 1263. The cross-correlation value for the alignment of Site 1265 to Site 1263 was 0.989, yielding a p-value of 0.000.
Section 3: Creating age models for Site 690, Site 1262, and Site 1265

In this section, age models are applied to Site 690, Site 1262, and Site 1265 records before and after they have been aligned to Site 1263. The age model used is obtained from Röhl et al. (2007). In this paper, they aligned records by identifying the precessional cycles of Fe, Ba, and Ca records. Ages are assigned at a number of depths at each of these different cites in Röhl et al. (2007). For our alignments, we have a “pre-warped” record, on a depth scale (Site 1262, Site 1265, or Site 690 depth scale). We also have an “aligned” record, on a Site 1263 depth scale. The age model assigned to the “pre-warped” record, corresponds to the ages assigned by Röhl et al. (2007) to depths in the candidate record (Site 1262, Site 1265, or Site 690). The age model assigned to the “aligned” record corresponds to the ages assigned by Röhl et al. (2007) to the Site 1263 depths. These ages essentially show the discrepancy between our alignment and Röhl et al. (2007) alignments.

In Figure S10, the comparison between the Site 690 age model applied to the “pre-warped” Site 690 record and Site 1263 age model applied to the “aligned” Site 690 record show that our DTW alignment compresses Site 690 in comparison to the alignment in Röhl et al., (2007), indicating a faster sedimentation rate. Figure S11, shows that our DTW alignment compresses the Site 1262 record overall, but also has a longer carbon isotope excursion. Figure S12, shows that our DTW alignment places the peak of the CIE later.
Figure S10: In gray, is the “pre-warped” Site 690 record with age obtained from the ages assigned to Site 690 depths in Röhl et al. (2007). In blue, is the “aligned” Site 690 record with age obtained from the ages assigned to Site 1263 depths in Röhl et al. (2007).
Figure S11: In gray, is the “pre-warped” Site 1262 record with age obtained from the ages assigned to Site 1262 depths in Röhl et al. (2007). In blue, is the “aligned” Site 1262 record with age obtained from the ages assigned to Site 1263 depths in Röhl et al. (2007).
Figure S12: In gray, is the “pre-warped” Site 1265 record with age obtained from the ages assigned to Site 1265 depths in Röhl et al. (2007). In blue, is the “aligned” Site 1265 record with age obtained from the ages assigned to Site 1263 depths in Röhl et al. (2007).
Section 4: Site 690 bulk record

Figure S13. Bulk $\delta^{13}$C record (black; Bains et al., 1999) and XRF-derived Fe intensity (grey; Rohl et al., 2007) from ODP Hole 690B overlying core photo. Blue numbers 2 through 5 indicate precession cycles identified by Rohl et al., 2007. Black numbers (with red arrows) indicate select major biotic and environmental events identified by Bralower et al. (2014): 1) initial surface warming identified from planktonic $\delta^{18}$O shift, 2) base of chemical erosion indicated by decreasing CaCO$_3$, 3) input of greenhouse gases indicated by planktonic $\delta^{13}$C shift, 4) peak surface warming indicated by planktonic $\delta^{18}$O, 5) thermocline CO$_2$ propagation indicated by thermocline $\delta^{13}$C shift, and 6) deep water dissolution indicated by foram fragmentation increase. Hatched interval indicates the gap identified by DTW in the bulk $\delta^{13}$C record.
Section 5: Sample DTW alignment of a target and candidate record

This section walks through a sample alignment of a candidate record to a target record using the DTW code. Text in red correspond to lines of code used in the DTW code in MATLAB.

A target record ‘x’ corresponds to a sample $\delta^{13}$C record in depth. And a candidate record ‘r’ corresponds to a sample $\delta^{13}$C record in depth.

\[x=\text{sample target record}\]

<table>
<thead>
<tr>
<th>Depth (m)</th>
<th>$\delta^{13}$C (vPDB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>30</td>
<td>5</td>
</tr>
<tr>
<td>40</td>
<td>2</td>
</tr>
<tr>
<td>50</td>
<td>3</td>
</tr>
</tbody>
</table>

\[r=\text{sample candidate record}\]

<table>
<thead>
<tr>
<th>Depth (m)</th>
<th>$\delta^{13}$C (vPDB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>2</td>
</tr>
<tr>
<td>65</td>
<td>4</td>
</tr>
<tr>
<td>90</td>
<td>1</td>
</tr>
<tr>
<td>95</td>
<td>2</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
</tr>
</tbody>
</table>
A matrix is first created that finds the squared difference between every data point for two series. In the below table, the numbers in the white boxes are the squared difference between the adjacent $\delta^{13}$C values in the gray boxes.

N is the number of total number of columns in the matrix, M is the total number of rows in the matrix. n is the matrix row number, m is the matrix column number.

\[
d=(\text{repmat}(x(:,1:M)-\text{repmat}(r(:,1:N,1)),^2);
\]

<table>
<thead>
<tr>
<th>x(Depth))</th>
<th>x($\delta^{13}$C (vPDB))</th>
<th>r($\delta^{13}$C(vPDB))</th>
<th>r(Depth)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>4  4</td>
<td>16  4</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>0  0</td>
<td>4  0</td>
</tr>
<tr>
<td>30</td>
<td>5</td>
<td>9  9</td>
<td>16  1</td>
</tr>
<tr>
<td>40</td>
<td>2</td>
<td>0  0</td>
<td>4  0</td>
</tr>
<tr>
<td>50</td>
<td>3</td>
<td>1  1</td>
<td>1  1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2  2</td>
<td>4  2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100  95</td>
<td>65  50</td>
</tr>
</tbody>
</table>

The squared difference matrix is then adjusted to account for the edge parameter, which in this example is chosen to be 0.5. Since the edge value is 0.5, the values along the top row, left-most column, right-most column, and bottom row are all multiplied by 0.5.

for \(d(m,n)\rightarrow m\) corresponds to the row number in the matrix, and \(n\) corresponds to the column number in the matrix. The colon sign means that the same thing is done for every row number or column number in the matrix.

\[
d(1,:)=d(1,:)*\text{edge};
\]

\[
d(:,end)=d(:,end)*\text{edge};
\]

\[
d(end,:)=d(end,:)*\text{edge};
\]

\[
d(:,1)=d(:,1)*\text{edge};
\]
\[
\begin{array}{|c|c|c|c|c|c|}
\hline
\text{x(\text{Depth})} & \text{x(\delta^{13}\text{C (vPDB)})} & 1 & 2 & 0.5 & 8 & 1 \\
\hline
10 & 0 & & & & & \\
20 & 2 & 0 & 0 & 1 & 4 & 0 \\
30 & 5 & 4.5 & 9 & 16 & 1 & 4.5 \\
40 & 2 & 0 & 0 & 1 & 4 & 0 \\
50 & 3 & 0.25 & 0.5 & 2 & 0.5 & 0.25 \\
\hline
\end{array}
\]

\[
\text{r(\delta^{13}\text{C (vPDB)})} \\
\text{r(\text{Depth})}
\]

% creating new cumulative difference matrix ‘D’ from d
D=zeros(size(d));
D(1,1)=d(1,1):

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
\text{x(\text{Depth})} & \text{x(\delta^{13}\text{C (vPDB)})} & 0 & 0 & 0 & 0 & 0 \\
\hline
10 & 0 & & & & & \\
20 & 2 & 0 & 0 & 0 & 0 & 0 \\
30 & 5 & 0 & 0 & 0 & 0 & 0 \\
40 & 2 & 0 & 0 & 0 & 0 & 0 \\
50 & 3 & 0.25 & 0 & 0 & 0 & 0 \\
\hline
\end{array}
\]

\[
\text{r(\delta^{13}\text{C (vPDB)})} \\
\text{r(\text{Depth})}
\]

% fill the the edges of the cumulative difference matrix, D
if 1,
for n=2:N
  D(n,1)=d(n,1)+D(n-1,1);
end
for m=2:M
  D(1,m)=d(1,m)+D(1,m-1);
end
end:

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
\text{x(\text{Depth})} & \text{x(\delta^{13}\text{C (vPDB)})} & 5.75 & 0 & 0 & 0 & 0 \\
\hline
10 & 0 & & & & & \\
20 & 2 & 4.75 & 0 & 0 & 0 & 0 \\
30 & 5 & 4.75 & 0 & 0 & 0 & 0 \\
40 & 2 & 0.25 & 0 & 0 & 0 & 0 \\
50 & 3 & 0.25 & 0.75 & 2.75 & 3.25 & 3.5 \\
\hline
\end{array}
\]

\[
\text{r(\delta^{13}\text{C (vPDB)})} \\
\text{r(\text{Depth})}
\]

\[
g \text{ (diagonal parameter)}=1.05
\]

% look two steps ahead
n=2:N;
for m=2:M
    % check the three preceding squares to determine square with minimum value and add this value to d
    D(n,m)=d(n,m)+min([g*D(n-1,m),D(n-1,m-1),g*D(n,m-1)]);
end
end

<table>
<thead>
<tr>
<th>x(Depth)</th>
<th>x(δ^{13}C (vPDB))</th>
<th>x(5)</th>
<th>y(5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>5.75</td>
<td>5.75</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>4.75</td>
<td>4.75</td>
</tr>
<tr>
<td>30</td>
<td>5</td>
<td>4.75</td>
<td>9.25</td>
</tr>
<tr>
<td>40</td>
<td>2</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>50</td>
<td>3</td>
<td>0.25</td>
<td>0.75</td>
</tr>
</tbody>
</table>

% start at the end point (N,M) and work your way back along the minimum path
Dist=D(N,M);
n=N;
m=M;
k=1;
w=[];
w(1:)=[N,M];
while ((n+m)==2)
    if (n-1)==0  % if you get to the start of the column, move over one row
        m=m-1;
    elseif (m-1)==0 % if you get to the start of the row, move over one column
        n=n-1;
    elseif (n-2)==0 & (m-2)==0 % if you get to the start of the diagonal
        n=n-1;
m=m-1;
    elseif (n-2)==0
        [~,number]=min([D(n-1,m),D(n,m-1),D(n-1,m-1),D(n,m-2) D(n-2,m)]);
        switch number
        case 1
            n=n-1;  % follow the path up a row
        case 2
            m=m-1;  % follow the path to the left
        case 3
            n=n-1;  % follow the diagonal path
            m=m-1;
        case 4
            m=m-2;  % follow the path to the left 2
        case 5
            n=n-1;  % follow the path to the left 2 and down 1
            m=m-2;
        end
    elseif (m-2)==0
        [~,number]=min([D(n-1,m),D(n,m-1),D(n-1,m-1),D(n,m-2) D(n-2,m-1)]);
        switch number

r(δ^{13}C(vPDB))
r(Depth)
case 1
  n=n-1;  % follow the path up a row
case 2
  m=m-1; % follow the path to the left
case 3
  n=n-1; % follow the diagonal path
  m=m-1;
case 4
  n=n-2; % follow the path to the down 2
case 5
  n=n-2; % follow the path to the left 1 and down 2
  m=m-1;
case 6
  % m=m-2; % follow the path to the left 2
  n=[n;n];
  m=[m-1;m-2];
case 7
  % n=n-1; % follow the path to the left 2 and down 1
  % m=m-2;
  n=[NaN;n-1];
  m=[m-1;m-2];
case 8
  % n=n-2; % follow the diagonal path 2
  % m=m-2;
  n=[n-1;n-2];
  m=[m-1;m-2];
case 9
  n=n-2; % follow the path to the left 2 and down 2
  m=m-1;
case 10
  % n=n-2; % follow the path down 2
  n=[n-1;n-2];
  m=[m;m];
end
end
k=k+1;
w=cat(1,w,[n,m]);

% extract the final value to step forward in time
n = n(end);
m = m(end);
end
Start at the top right corner and draw a path through the minimum values. These highlighted values show the warping path dictating how the candidate record aligns to the target record.

<table>
<thead>
<tr>
<th>x(Depth))</th>
<th>x($\delta^{13}\text{C (vPDB)}$)</th>
<th>r($\delta^{13}\text{C(vPDB)}$)</th>
<th>r(Depth)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0</td>
<td>5.75</td>
<td>3.375625</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>4.75</td>
<td>2.2625</td>
</tr>
<tr>
<td>30</td>
<td>5</td>
<td>4.75</td>
<td>2.2625</td>
</tr>
<tr>
<td>40</td>
<td>2</td>
<td>0.25</td>
<td>2.2625</td>
</tr>
<tr>
<td>50</td>
<td>3</td>
<td>0.25</td>
<td>3.5</td>
</tr>
</tbody>
</table>

The figure below is a visual representation of the alignment of the candidate record ‘r’ to the target record ‘x’.
CURRICULUM VITAE

Seyi Ajayi

Education

The Pennsylvania State University Aug 16-Dec 20
Doctor of Philosophy: Geosciences
Dissertation: Examining the Fidelity of Carbon Isotope Records in the PETM

The Pennsylvania State University Aug 14-Aug 16
Master of Science: Geosciences
Thesis: Testing the Viability of Supercritical Carbon Dioxide as a Fracking Fluid by Computing its Chemical Interaction with Illite

The Pennsylvania State University Aug 10-May 14
Bachelor of Science: Chemical Engineering

Awards Received

AAPG Imperial Barrel Award Runner-Up, Participated in the AAPG Imperial Barrel Award competition; participated on a team that won the Eastern Section and advanced to finish second place in the international competition; 143 schools participated from 40 different countries; the competition teams up four or five students from a university and provides them with a dataset to analyze the petroleum potential of a given basin; the findings are then given in a 25-minute presentation to a panel of high-level industry executives (Feb 16-Jun 16)

Scholarships

Shell PGI Student Fellowship, Received a scholarship provided by Shell as part of the Petroleum Geosystems Initiative (Aug 14-May 16)
Bunton-Waller Fellowship, Received a Bunton-Waller Fellowship; program is intended to attract students from various ethnic and cultural backgrounds who demonstrate high academic potential (Aug 14-May 16)

Publications
