Assessing coral Sr/Ca-SST calibration techniques using the species *Diploria strigosa*

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Abstract

The coral species *Diploria strigosa* is a promising archive for paleoclimate reconstruction in the tropical Atlantic, but limited work has been accomplished thus far to quantify the relationship between strontium to calcium ratios and sea surface temperatures in this species. In this study, we collected three modern *D. strigosa* coral colonies from Anegada, British Virgin Islands to refine the use of this species as a paleoclimate archive. Three regression techniques including ordinary least squares, reduced major axis, and weighted least squares were used to assess how assumptions implicit in these regression methods influence the calibration. Our analysis demonstrated that regression slopes were strongly impacted by the assumptions about data uncertainty. We recommend using the unbiased weighted least squares regression technique for calibrating the Sr/Ca paleothermometer, especially when precise local sea surface

temperature data are unavailable. Combining our Sr/Ca data with previously published data from this species results in a multi-site, multi-colony temperature sensitivity of $-0.046(\pm < 0.001)$ mmol/mol/°C for mean-centered monthly data, $-0.059(\pm 0.001)$ mmol/mol/°C for monthly anomalies, and $-0.063(\pm 0.004)$ for annual anomalies. We suggest these relationships are the best available characterization of the temperature dependence of Sr/Ca in *D. strigosa*, and can be utilized in future paleoclimate reconstructions.

Keywords: *Diploria strigosa*; Sr/Ca; Calibration; Weighted least square

1 **1 Introduction**

2 A few key genera of reef-building corals are used in most paleoclimate studies to
3 reconstruct tropical sea surface temperature (SST) [Corrège, 2006; DeLong *et al.*, 2007;
4 Saenger *et al.*, 2008]. *Porites* is the genus most often used in the Pacific [e.g., Corrège,
5 2006; Gagan *et al.*, 2012; McGregor and Gagan, 2003; Shen *et al.*, 1996], whereas the
6 *Montastraea annularis* species complex (now formally assigned to the genus *Orbicella*,
7 [Budd *et al.*, 2012]) is commonly used in the Atlantic [e.g., Kilbourne *et al.*, 2008;
8 Saenger *et al.*, 2008; Smith *et al.*, 2006; Swart *et al.*, 2002; Watanabe *et al.*, 2001;
9 Watanabe *et al.*, 2002].

10 The genus *Diploria* is another abundant massive coral genus commonly found
11 growing on Atlantic reefs but it has been used much less extensively for paleoclimate
12 research. Initial work on the genus *Diploria* primarily focused on slow growing
13 specimens of the species *D. labyrinthiformis* from Bermuda [Cohen and Thorrold, 2007;
14 Cohen *et al.*, 2004; Draschba *et al.*, 2000; Goodkin *et al.*, 2007; Goodkin *et al.*, 2005;
15 Kuhnert *et al.*, 2002]. The corals used in these studies had annual growth rates in the 2-5
16 mm range and many researchers noted a significant impact of coral growth rates on
17 geochemistry in these slow-growing specimens [Cardinal *et al.*, 2001; Cohen *et al.*, 2004;
18 Goodkin *et al.*, 2007; Goodkin *et al.*, 2005]. Cohen and Thorrold [2007] recommended
19 extremely fine sampling of this species to minimize the impact of biosmoothing [Gagan
20 *et al.*, 2012] and time-transgressive sampling on climate reconstructions. Alternatively,
21 Goodkin *et al.* [2007] suggested a growth-corrected calibration based on three different

corals. The goal of their study was to provide a universal calibration that could be applied generally to *D. labyrinthiformis*, both modern and fossil specimens.

Research on the species *D. strigosa* is not as well developed as for *D. labyrinthiformis*. *Hetzinger et al.* [2006] published a 41-year Sr/Ca-SST calibration for a fast growing *D. strigosa* from Guadaloupe, and suggested that *D. strigosa* was a promising archive of Atlantic SST information. They pointed out that faster growth rates in their coral specimen led to less time integration of the sub-samples than with the slower-growing specimens of *D. labyrinthiformis* examined to date (see [*Sadler et al.*, 2014] and their figure 4 for an excellent explanation of the relevant skeletal geometry). Three subsequent studies utilized Hetzinger's calibration, citing it as the best available calibration for this species [*Giry et al.*, 2010; *Giry et al.*, 2012; *Hetzinger et al.*, 2010]. *Giry et al.* [2010] investigated the sub-millimeter scale Sr/Ca heterogeneity in a specimen of *D. strigosa*. Their results supported the conclusion by *Hetzinger et al.* [2006] that time integration of drilled samples is much less in these faster-growing specimens than in the slow-growing *D. labyrinthiformis*. Additionally, *Giry et al.* [2010] suggested that micro-milling the thecal wall with a fine (0.6 mm) drill bit was the best method for extracting a climate signal from this species to avoid skeletal elements with strong non-climatic Sr/Ca signals.

In this study we further refine the use of this species for paleoclimate reconstructions. *Hetzinger et al.* [2006] defined the Sr/Ca-temperature slope in *D. strigosa* using a single coral colony, but as *Goodkin et al.* [2007] pointed out, multi-colony calibrations are inherently more accurate for paleoclimate reconstructions than those that use individual coral specimens selected from a population. In this study, we

explore calibration slopes from multiple modern corals and combine them to provide a more robust Sr/Ca-SST calibration for this species. We utilize new data from multiple specimens of *D. strigosa* which grew offshore from the island of Anegada, British Virgin Islands, in the northern Caribbean, and combine it with existing data from specimens which grew offshore from Guadeloupe [Hetzinger *et al.*, 2006] and Bonaire [Giry *et al.*, 2012], to create a regionally applicable calibration slope.

Most prior calibration studies used the Ordinary Least Squares (OLS) regression technique, which has been shown to have limitations derived from implicit assumptions about measurement errors [Solow and Huppert, 2004]. In this study, we explore the use of OLS and compare it to other methods that have been recommended as alternates, such as Reduced Major Axis (RMA) regression [Quinn and Sampson, 2002; Nurhati *et al.*, 2009] and Weighted Least Squares (WLS) [DeLong *et al.*, 2007; DeLong *et al.*, 2011; DeLong *et al.*, 2014; Thirumalai *et al.*, 2011]. We compare multiple calibration techniques with the same data to assess how assumptions implicit in different regression methods influence the resulting calibration slopes and we provide our best estimate of the Sr/Ca-temperature sensitivity for this coral species.

2 Data and Methods

2.1 Sampling

The coral samples used in this study were collected as hand samples in March 2013 from the beach berm at Soldier Point, Anegada (Figure 1). Beach berm deposits of coral boulders are common on high-energy coastlines in reef-growing areas and they

provide a near unlimited supply of short (decades-long) coral records from a variety of time periods. We collected pristine-looking coral boulders with the goal of creating a replicated 20th century calibration without any damage to living coral colonies, minimizing the ecological impact of our paleoclimate research.

Approximately 5 cm diameter cores were drilled from each of the three coral boulders in the field. The cores were designated 13AN17, 13AN18, 13AN19 and were cut along the growth direction into approximately 5 mm thick slabs using a tile saw dedicated to cutting coral cores. Each slab was individually immersed in a clean plastic container with deionized water and ultrasonicated for 30 minutes. Following a rinse in deionized water, the samples were air-dried and stored covered with clean Kimwipes®.

Figure 1. Samples for this study were obtained from a beach berm deposit at Soldier Point on the north side of Anegada, British Virgin Islands. This carbonate island lies on the border between the Caribbean Sea and the tropical North Atlantic. Buoy-based SST data discussed in the paper came from Charlotte Amalie harbor on St. Thomas in the U.S. Virgin Islands.

Coral slabs were drilled using a computer-controlled micromilling system, equipped with a 0.5-mm diameter carbide steel dental drill bit. Before drilling the coral

slabs, annual extension rates were estimated by measuring the distance between ten density band couplets. The targeted sampling resolution was 12 samples per year. Sub-samples of skeletal powder were extracted carefully at a constant sampling depth of 0.5 mm per sub-sample along the center of the thecal wall, to obtain the best chronology and environmental signal possible [Giry *et al.*, 2010]. Thin-section billets were cut adjacent to the micro-sampling paths in each core. No evidence of secondary aragonite or calcite were found in the thin sections.

2.2 Coral Sr/Ca

Sr/Ca ratios in the coral aragonite were measured using a Perkin Elmer Optima 8300 Inductively Coupled Plasma Optimal Emission Spectrometer (ICP-OES) at the University of Maryland Center for Environmental Science, Chesapeake Biological Laboratory campus. We weighed 150 ± 50 μg coral powder from each sample and dissolved it in different volumes (2–4 mL) of 2% trace-metal grade nitric acid to bring the concentration of calcium to ~ 20 ppm. Calibration standards with known calcium and strontium concentrations were used to convert instrumental signal intensity to sample concentration. Reference standards were measured before and after each sample to calculate an instrumental drift correction to be applied to the data, as per Schrag [1999]. The calcium and strontium concentrations of the reference standards were similar to the samples, with values of ~ 20 ppm and 400 ppb, respectively. An in-house laboratory coral standard prepared from an *Orbicella faveolata* coral dissolved in 2% trace-metal grade nitric acid to similar calcium concentration as the samples provided an independent check of analytical precision and accuracy. The Sr/Ca ratios of these two standards were cross calibrated with ICP-OES instruments at the University of Texas at Austin

Analytical Laboratory for Paleoclimate Studies and the US Geological Survey in St. Petersburg, Florida. Long-term analytical precision for the reference standard solution is 0.12% (2σ , 0.011 mmol-Sr/mol-Ca, $n = 4475$). Long-term analytical precision for the coral standard solution is 0.26% (2σ ; 0.023mmol-Sr/mol-Ca, $n = 578$). These estimates of analytical precision are used to estimate the uncertainty of the Sr/Ca data in our regression analysis. Applying a Sr/Ca–temperature relationship of 0.042 mmol/mol/°C from *Hetzinger* [2006] to the 2σ standard deviations of the reference and coral solutions results in estimated temperature standard errors on individual data points of 0.26°C and 0.55°C for reference standard solution and coral standard solution, respectively.

2.3 Coral Chronology

In this study, the age of the corals was determined by a combination of uranium-series dates, X-radiographs, and correlations of coral Sr/Ca to SST. Sub-samples weighing on average 600 ± 200 mg and representing approximately one year of coral growth were cut from coral slabs 13AN17 and 13AN18 for U-series analysis. 13AN19 was not subsampled for U-series dating because initially we planned not to use the extremely short core. Uranium-series analysis was undertaken on these sub-samples at the High-Precision Mass Spectrometry and Environment Change Laboratory at National Taiwan University. The wet chemistry was performed following *Shen et al.* [2003] on the 15th of September, 2013 and instrumental analysis was performed by using Multicollector-Inductively Coupled Plasma-Mass Spectrometry (MC-ICP-MS) following *Shen et al.* [2012].

X-radiographs taken at the United States Geological Survey in St. Petersburg, Florida, were used to reveal the annual density band couplets for age modeling. The

positions of the dated coral pieces were identified on the X-radiographs and an initial depth/age relationship determined by annual density band counting from the position and date indicated.

The conversion of the Sr/Ca data from depth domain to time domain was achieved by matching coral Sr/Ca seasonal cycles to SST seasonal cycles using AnalySeries software (available through NOAA's National Climate Data Center at <http://www.ncdc.noaa.gov/data-access/paleoclimatology-data/datasets/software>) [Paillard *et al.*, 1996]. The SST record used for alignment is the $2^{\circ} \times 2^{\circ}$ gridded Extended Reconstructed Sea Surface Temperature (ERSST) version 3b data [Smith *et al.*, 2008] centered on 19°N, 64°W. The time-domain Sr/Ca ratios were re-sampled to monthly intervals and provide the primary data used in comparisons with monthly SST time series data. Annual growth rates were calculated from two successive winters in each annual cycle as defined by the depth-domain Sr/Ca data.

Combining the U-series dates, density banding from the X-rays, and Sr/Ca seasonal cycles matched to seasonal SST resulted in data organized in relative time but lacking a firm date because of the uncertainty in the U-series dates for each sample. We correlated the Sr/Ca anomalies to lagged SST anomalies over a range of time lags around the U-series uncertainty to further narrow the age of the samples. Note that we compared Sr/Ca measured in coral 13AN19 with the values measured in coral 13AN17 to determine the age of 13AN19 because their stratigraphic position and degree of surface weathering (none) in the field indicated that they likely washed ashore in the same storm. The strongest correlation in a lagged correlation analysis of coral 13AN19 Sr/Ca and SST over a wide range of time confirmed the age of 13AN19.

2.4 Instrumental Data

National Oceanic and Atmospheric Administration/National Climatic Data Center (NOAA/NCDC) ERSST v.3b [Smith et al., 2008] is the major temperature data source we used for the Sr/Ca-SST calibrations. The temporally and spatially complete ERSST data were created by interpolating between gaps in the instrumental database [Smith and Reynolds, 2004] and in many locations gridded data products like this one are the only data available for comparing with modern coral geochemical data. Gridded data products like ERSST do not always capture fine-scale temperature variations that a coral may experience at the local level, so we also compared the gridded data with both a higher resolution ($0.25^\circ \times 0.25^\circ$) satellite-derived Optimum Interpolation SST (OISST v.2) [Reynolds et al., 2007] and NOAA National Data Buoy Center SST measurements from Charlotte Amalie, US Virgin Islands, about 75km from Soldier Point, Anegada (Figure 1). The ERSST and OISST data over 1981-2012 are highly correlated on monthly scales ($r = 0.98, p < 0.01, n = 376$). Note that the variances of the ERSST and OISST data are 1.18 and 1.13, respectively. The average absolute difference between the records is 0.27°C . The available buoy data (from 2005-2012) are also highly correlated with ERSST data on monthly scales ($r = 0.85, p < 0.01, n = 73$). The variance of available buoy data is 1.89, which is higher than the variances of large-scale gridded data. The average absolute difference between buoy data and ERSST data is 1.45°C , which is also much higher than the difference between OISST and ERSST data.

2.5 Statistical Methods

The salient features of the two regression techniques most commonly used in coral-paleoclimate work, OLS and RMA are compared in the following paragraphs, with

a subsequent description of WLS and a bootstrapping procedure we developed for this study to estimate the uncertainty of our calibrations.

OLS is a generalized linear modeling technique that regresses a response variable on a predictor variable [Cavalli-Sforza and Edwards, 1967]. This technique minimizes the sum of squared vertical distances between the observed response variables and the predicted variables [Cavalli-Sforza and Edwards, 1967]. RMA is also a least-squares method but differs from OLS in that it uses a different definition for the residuals. It accounts for potential errors in both variables simultaneously by minimizing the distance perpendicular to the regression line [Clarke, 1980].

The primary difference between OLS and RMA is that RMA assumes equal error variances exist in both the dependent variable and the independent variable, while OLS only accounts for errors in the dependent variable [Smith, 2009]. The resulting difference in regression lines is that OLS regression lines are asymmetric, i.e., dependent on which variable is on the x-axis. However, the RMA regression lines are symmetric with respect to inversion of the axes. It has been pointed out that OLS regressions for paleoclimate reconstructions produce a biased estimate of SST due to the presence of errors in SST used in the calibration [Delong *et al.*, 2007; Solow and Huppert, 2004]. Solow and Huppert [2004] recommended a bias correction and Delong *et al.* [2007] recommended Maximum Likelihood Estimation regression technique instead, but to the best of our knowledge, few studies have yet incorporated these recommendations.

Fitch and Margoliash [1967] suggested the Weighted Least Squares (WLS) method to account for uncertainty in both independent and dependent variables for regressions in general. In this technique, each term includes an additional weight

determining how much each observation in the data set influences the final parameter estimates. The weights for each point are assigned by the reciprocal of the estimated uncertainty in both variables, Sr/Ca and SST in this case. Less weight is given to the less precise measurements and more weight to more precise measurements.

WLS has been suggested as a more robust alternative to OLS in situations where there is the potential for error in both regression variables and for correlated errors in both regression variables [York *et al.*, 2004]. WLS minimizes the weighted sum-of-squares, accounting for estimated errors and covariance in both dependent and independent variables [Fitch and Margoliash, 1967]. York *et al.* [2004] put forth a method for calculating the standard errors on the slope and intercept for WLS regression that makes the method exactly equal to Maximum Likelihood Estimation regression favored by the statistics community. The slope, intercept, and standard errors of regressions in this study were calculated following [York *et al.*, 2004] using the MATLAB code provided in [Thirumalai *et al.*, 2011].

We used the 2-sigma percent analytical precision of our coral standard (0.26%) multiplied by each Sr/Ca determination to estimate Sr/Ca uncertainty. The SST uncertainty estimates provided with the ERSST v3b data served for estimating the SST uncertainty.

Additionally, we developed a bootstrap method with weighted least squares (BWLS) to iteratively determine the range of calibrations possible from a given dataset. In our BWLS technique, 75% of the data were randomly selected 1000 times and each selection was analyzed using the WLS technique [York *et al.*, 2004]. Each random selection leaves out 25% of the data that can be used to evaluate the calibration. In

contrast to the errors for OLS, RMA, and WLS, which are calculated from a single calibration, the BWLS calibration technique uses the 1000 WLS regression slopes to estimate the 95% confidence interval on the value of the regression slope according to equation 2.4 in Efron and Tibshirani [1986].

The BWLS technique determines the range of regression lines that can be obtained from the regression data and allows us to estimate how results may differ if we were to do the calibration multiple times with data that have the same underlying Sr/Ca-SST relationship and error structure. It results in an estimate of the uncertainty in the regression slope that is based on the actual data, compared with standard methods that make assumptions about the data distribution and error structure.

A complicating factor for multi-colony calibrations is that differences in mean Sr/Ca values have been found in some *Diploria strigosa* corals growing on the same reef at the same time that seem unrelated to temperature [Giry *et al.*, 2012]. This study uses two approaches to compensate for potential mean shifts with Sr/Ca data from three colonies. The approaches are to (1) center the data before regression by removing the mean Sr/Ca value of each coral colony and removing the mean SST value, and (2) regress using the Sr/Ca and SST anomalies i.e., remove the average annual cycle in Sr/Ca and SST time series.

3 Results

3.1 Age Model

Corals 13AN17, 13AN18, and 13AN19 grew 18, 28, and 10 years with extension rates ($\pm$ standard error) of $6.9(\pm 0.4)$ mm/yr, $5.6(\pm 0.2)$ mm/yr, and $6.2(\pm 0.4)$ mm/yr

respectively, reflected in the regular annual density bands visible in the X-radiographs of the coral slabs (Figure 2). Uranium-series dates for corals 13AN17 and 13AN18 (Table 1) are 1989.5 ± 0.58 CE and 1953.3 ± 0.72 CE, respectively. Correlating the Sr/Ca anomalies to SST anomalies over a range of time lags around the U-series uncertainty leads us to conclude that the cores 13AN17 and 13AN18 represent coral growth from 1990-2008 and 1948-1977 respectively. The minimum lagged correlation of 13AN19 Sr/Ca to instrumental SST over the 20th century led us to assign an age range of 1997-2008 to this coral.

Table 1. U-Th isotopic compositions and ^{230}Th ages for subsamples of coral slabs, 13AN17 and 13AN18, collected from Anegada, British Virgin Islands.

Sample ID	Weight (g)	^{238}U (ppb)	^{232}Th (ppt)	$\delta^{234}\text{U}$ Measured ^a	$[\text{}^{230}\text{Th}/\text{}^{238}\text{U}]$ Activity ^c	$[\text{}^{230}\text{Th}/\text{}^{232}\text{Th}]$ ppm ^d	Age Uncorrected	Age Corrected ^{c,e}	$\delta^{234}\text{U}$ Initial Corrected ^b
13AN17	0.1794	1914.1 $\pm$ 2.0	34.3 $\pm$ 2.6	148.9 $\pm$ 1.7	0.000254 $\pm$ 0.000006	234 $\pm$ 18	24.12 $\pm$ 0.54	23.71 $\pm$ 0.58	148.9 $\pm$ 1.7
13AN18	0.1938	2041.1 $\pm$ 2.2	27.6 $\pm$ 2.4	147.4 $\pm$ 1.7	0.000634 $\pm$ 0.000007	775 $\pm$ 68	60.31 $\pm$ 0.70	59.99 $\pm$ 0.72	147.4 $\pm$ 1.7

^a $\delta^{234}\text{U} = ([\text{}^{234}\text{U}/\text{}^{238}\text{U}]_{\text{activity}} - 1) \times 1000$.

^b $\delta^{234}\text{U}_{\text{initial}}$ corrected was calculated based on ^{230}Th age (T), i.e., $\delta^{234}\text{U}_{\text{initial}} = \delta^{234}\text{U}_{\text{measured}} \times e^{\lambda^{234}T}$, and T is corrected age.

^c $[\text{}^{230}\text{Th}/\text{}^{238}\text{U}]_{\text{activity}} = 1 - e^{-\lambda^{230}T} + (\delta^{234}\text{U}_{\text{measured}}/1000)[\lambda_{230}/(\lambda_{230} - \lambda_{234})](1 - e^{-(\lambda_{230} - \lambda_{234})T})$, where T is the age.

^d The degree of detrital ^{230}Th contamination is indicated by the $[\text{}^{230}\text{Th}/\text{}^{232}\text{Th}]$ atomic ratio instead of the activity ratio.

^e Age corrections for samples were calculated using an estimated atomic $^{230}\text{Th}/\text{}^{232}\text{Th}$ ratio of 4 ± 2 ppm [Shen *et al.*, 2008].

Figure 2. X-radiographs of the corals used in this study. Raw Sr/Ca-depth plots are displayed on the X-radiographs with high Sr/Ca values towards the left.

3.2 Coral Strontium-Calcium Ratios

The monthly Sr/Ca ratios displayed strong seasonal variation (Figure 3). The mean and standard deviation of the coral skeletal Sr/Ca in the three cores 13AN17, 13AN18, and 13AN19 were 8.99 ± 0.06 mmol/mol, 9.13 ± 0.06 mmol/mol, and 8.95 ± 0.06 mmol/mol, respectively. The standard deviation of each time series is controlled by the range of the seasonal cycle and can be thought of as a measure of the seasonal Sr/Ca range in each coral. Periods of maximum Sr/Ca ratios correspond to low-density bands and minimum Sr/Ca ratios correspond to high-density bands, consistent with high-density bands forming in the warm boreal summer and low-density bands forming during the

relatively cool winter as found in *Orbicella faveolata* at this latitude [Watanabe *et al.*, 2002, Kilbourne *et al.*, 2008]. Standards run with the samples show no similar offsets indicating the mean differences between corals are not an analytical artifact, but represent true population-scale variations in mean skeletal Sr/Ca.

Figure 3. Reconstructed SST anomalies from modern corals by using mean-centered Sr/Ca records. From top to bottom the panels represent coral 13AN17, 13AN18, and 13AN19,

respectively. Solid lines represent the Sr/Ca (left axis) and Sr/Ca-based SST anomalies (right axis). Dashed lines represent the gridded SST. Coral Sr/Ca-derived SST anomaly was calculated using the OLS regression slope of $-0.048 \text{ mmol/mol/}^{\circ}\text{C}$ from this study.

3.3 Calibration of Sr/Ca with SST

First we report the results of the mean-centered data regressions. Within a colony, the three least squares regression techniques, OLS, WLS and BWLS, produced similar Sr/Ca-SST regression slopes, but the slope of the RMA regression in each coral colony is different from the Sr/Ca-SST regression slopes determined with the other regression techniques (Table 2). The regression slopes differ slightly between colonies no matter what regression technique is applied (Table 2). Similar to the results for the individual corals, when the data from all three corals are centered and combined, the ordinary least squares and weighted least squares methods give similar results, but the RMA regression is significantly different (Table 2, Figure 4).

We repeat these four different calibration techniques with 0.3°C , 0.5°C and 1.0°C estimated errors on all the temperature measurements to demonstrate the sensitivity of the calculated slopes to the ratio of uncertainty in the regression variables. The results show that the BWLS slope is closer to that obtained by OLS when the temperature uncertainty is small (average SST uncertainty 0.15°C , Figure 4a), consistent with the OLS assumption of zero error in the x-axis variable. The BWLS slope is similar to that obtained by RMA when the temperature uncertainty is about $\sim 0.5^{\circ}\text{C}$, consistent with the estimated uncertainty of our Sr/Ca data (0.023 mmol/mol or $\sim 0.5^{\circ}\text{C}$) and the RMA assumption of equal error in x and y variables. The BWLS becomes steeper as the estimated temperature uncertainty increases (Figure 4 b and c), indicative of the increased

relative uncertainty in the x-axis variable. Flipping the regression so that the dependent regressor is Sr/Ca instead of SST would result in effectively the same relationships between RMA and WLS because neither method is sensitive to the choice of dependent variable. However, OLS would plot as a mirror image of the current line across the RMA axis in Figure 4.

Table 2. Summary of Sr/Ca-SST relationships between the mean-centered Sr/Ca time series and ERSST data in three modern corals. Units on the regression slopes are mmol/mol/°C. The regression equation for the BWLS technique represents the average of all bootstrap regressions.

Regression Method	13AN17	13AN18	13AN19	All corals
OLS	-0.043±0.003	-0.052±0.002	-0.047±0.002	-0.048±0.001
RMA	-0.053±0.002	-0.059±0.002	-0.053±0.002	-0.056±0.001
WLS	-0.046±0.002	-0.054±0.001	-0.048±0.002	-0.050±0.001
BWLS	-0.046±0.001	-0.054±0.001	-0.048±0.001	-0.050±0.001

Figure 4. Regression lines determined by applying OLS, RMA, and WLS techniques to mean-centered Sr/Ca and mean-centered ERSSTs. Estimated errors in SST come from NOAA/NCDC ERSSTv.3b dataset [Smith *et al.*, 2008]. The grey points with error bars (2SE) represent data points in all three coral cores from Anegada.

A weakness of calibrating monthly mean-centered Sr/Ca data to SST is that the regression results are strongly controlled by the seasonal cycle [Crowley *et al.*, 1999; DeLong *et al.*, 2007] and may be influenced by sub-annual skeletal thickening [Gagan *et al.*, 2012]. To get around this issue, we repeated the regression analysis on the Sr/Ca and SST monthly anomalies. The correlation between Sr/Ca anomalies and SST anomalies are not significant at the 95% confidence level in all three modern corals, though the

correlation becomes significant when the data from all three corals are combined (Table 3).

The anomaly data produced a wide range of Sr/Ca-SST relationships, between 0.25 mmol/mol/°C and 0.89 mmol/mol/°C. Unlike the results obtained using the mean-centered data, regression analysis with anomaly data produced Sr/Ca-SST slopes that are statistically different depending on regression technique (Table 4, Figure 5). Only the WLS and related BWLS results were the same. Similar to the set of regressions on mean-centered data, the slopes of the RMA regressions are higher than the slopes of the other regressions. The large difference in regression equations shows the importance of assumptions about the distribution of error in the data when the signal-to-noise ratio is small as is the case with the monthly anomaly data.

We also repeat these four different calibration techniques on the combined three-coral dataset with 0.2, 0.25, and 0.3°C errors on the temperature measurements to demonstrate the sensitivity of the slope to statistical method and temperature uncertainty when using Sr/Ca and SST anomalies. The results are similar to the parallel experiment on the mean-centered data with the average BWLS slope increasing with increasing uncertainty in temperature measurements (Figure 5). However with the lower signal to noise ratio in the anomaly data, the calculated slopes are much more sensitive to the temperature uncertainty. The BWLS regression shows more variance with larger SST errors. As with the mean-centered regressions, the BWLS slope is more similar to that obtained with OLS when the temperature uncertainty is small (Figure 5a and b). Increasing the temperature uncertainty to only 0.25 increases the BWLS slope to a value similar to that obtained by RMA (Figure 5c). When the errors in temperature are larger

than 0.25°C, the BWLS method estimates a much steeper slope than either of the other methods (Figure 5d).

Table 3. Correlation coefficients between Sr/Ca anomalies and ERSST temperature anomalies in modern corals at this site.

	AN17	AN18	AN19	All
Correlation coefficients (r)	−0.44	−0.30	−0.53	−0.38
p-value	>0.05	>0.05	>0.05	<0.05
Number of data points (N)	217	347	214	688

Table 4. Summary of Sr/Ca-SST relationships between the Sr/Ca and ERSST monthly anomaly data in three modern corals. Units on the regression slopes are mmol/mol/°C. The regression equation for the BWLS technique represents the average of all bootstrap regressions.

Regression Method	13AN17	13AN18	13AN19	All corals
OLS	-0.043±0.006	-0.025±0.004	-0.047±0.007	-0.034±0.003
RMA	-0.098±0.006	-0.081±0.004	-0.053±0.007	-0.089±0.003
WLS	-0.069±0.006	-0.043±0.004	-0.067±0.007	-0.056±0.003
BWLS	-0.069±0.004	-0.043±0.003	-0.067±0.005	-0.056±0.002

Figure 5. Regression lines determined by applying OLS, RMA, and BWLS techniques to Sr/Ca anomalies and ERSST anomalies. The black points with error bars (2SE) represent data points in all three coral cores from Anegada.

Another method to remove the influence of the seasonal cycle is to calibrate with centered mean annual data. Different from the monthly anomaly data, the correlation between annual mean Sr/Ca and SST anomalies are significant at the 95% confidence level in 13AN17, 13AN18 and the combined data from all three corals, though the correlation becomes insignificant in coral 13AN19 (Table 5), likely because of the short length of the core. A plot of the data (Figure 6) shows much higher signal to noise ratio compared to the anomaly data regression analysis. However, the calculated regression slopes (Table 6) have larger error bars because of the reduced number of data points.

Notably the BWLS regression using annual data with all of the corals from Anegada (-0.052 ± 0.006 mmol/mol/°C) is nearly identical to the slope calculated with seasonal data (-0.050 ± 0.001 mmol/mol/°C).

Table 5. Correlation coefficients between annual mean Sr/Ca anomalies and ERSST temperature anomalies in modern corals at this site.

	AN17	AN18	AN19	All
Correlation coefficients (r)	-0.70	-0.38	-0.53	-0.51
p-value	<0.05	<0.05	>0.05	<0.05
Number of data points (N)	17	28	10	55

Table 6. Summary of Sr/Ca-SST relationships between the Sr/Ca and ERSST annual anomaly data in three modern corals. Units on the regression slopes are mmol/mol/°C. The regression equation for the BWLS technique represents the average of all bootstrap regressions.

Regression Method	13AN17	13AN18	13AN19	All corals
OLS	-0.062 ± 0.017	-0.028 ± 0.013	-0.047 ± 0.027	-0.041 ± 0.010
RMA	-0.090 ± 0.016	-0.074 ± 0.013	-0.089 ± 0.024	-0.081 ± 0.009
WLS	-0.070 ± 0.023	-0.039 ± 0.017	-0.050 ± 0.033	-0.052 ± 0.013
BWLS	-0.070 ± 0.010	-0.040 ± 0.009	-0.051 ± 0.010	-0.052 ± 0.006

Figure 6. Regression lines determined by applying OLS, RMA, WLS, and BWLS technique to annual mean Sr/Ca and ERSST data.

We combined the data collected from Anegada with existing data from Guadeloupe [Hetzinger *et al.*, 2006] and Bonaire [Giry *et al.*, 2012] to create a bulk calibration slope for *D. strigosa* in Caribbean. The resulting slope from the multi-site calibration using the BWLS technique was $-0.046(\text{SE} < 0.001)$ mmol/mol/°C for mean-centered data (Figure 7), $-0.059(\pm 0.001)$ mmol/mol/°C for monthly anomalies (Figure 8), and $-0.063(\pm 0.004)$ for annual anomalies (Figure 9).

Figure 7. Regression lines determined by applying the BWLS technique to mean-centered Sr/Ca and mean-centered ERSST data from multiple sites including Anegada, Guadeloupe, and Bonaire.

Figure 8. Regression lines determined by applying the BWLS technique to Sr/Ca anomalies and ERSST anomalies from Anegada, Guadeloupe, and Bonaire.

Figure 9. Regression line determined by applying the BWLS technique to annual Sr/Ca anomalies and annual ERSST anomalies from Anegada, Guadeloupe, and Bonaire.

The data left out of each regression iteration in our bootstrapped-WLS regression provides regression-independent data to assess reconstruction errors. For each iteration of the regression, the derived Sr/Ca–SST slope is applied to these regression-independent data and the calculated SSTs compared to instrumental SST. For the 3-coral Anegada regressions 95% of the monthly SST reconstructions are within $\pm 1.2^{\circ}\text{C}$ of the instrumental temperature, providing a 95% confidence level that can be assigned to a reconstructed temperature. Similar analysis of the Anegada monthly anomaly and annual data results in confidence intervals of $\pm 1.0^{\circ}\text{C}$ and 0.8°C , respectively. 95% confidence

intervals for reconstructed temperatures using all 5 corals are ± 1.3 , ± 1.0 , and ± 0.7 °C for monthly, monthly anomaly and annual data respectively.

4 Discussion

4.1 Mean Differences

The corals in this study have different mean Sr/Ca ratios that cannot be explained by differences in mean temperature at the time of coral growth according to the gridded temperature data. Mean differences between cores in this situation have multiple potential causes including: 1) the corals may have grown on different parts of the reef that may have had different temperatures (such as at different depths), 2) they may have grown on different parts of the reef with different mean seawater Sr/Ca, and 3) biological factors may have influenced the mean Sr/Ca. Although many studies have demonstrated the consistency of Sr/Ca ratios among *Porites lutea* and *Siderastrea siderastrea* coral colonies [DeLong *et al.*, 2007; DeLong *et al.*, 2011; DeLong *et al.*, 2014; Stephans *et al.*, 2004], there is some evidence that different coral colonies growing near each other can have colony-specific offsets in mean Sr/Ca ratios [DeLong *et. al.*, 2011; de Villiers *et al.*, 1994].

No significant relationship was found between annual Sr/Ca and growth rate in each coral colony, though it is possible that the mean shift of the growth rates in these three modern corals are responsible for the mean shift of the Sr/Ca ratios (Table 7). The relatively high Sr/Ca ratios and relatively low growth rates in coral 13AN18, compared to the other modern corals, is consistent with previous studies that suggest slower growing

Diploria colonies have higher Sr/Ca ratios [Goodkin *et al.*, 2005]. Without benefit of an array of thermistors monitoring SST variability on the reef and a water sampling program to ensure no seawater Sr/Ca changes could be impacting our site, we conclude that the cause of mean shifts in coral colony Sr/Ca ratios is ambiguous at this time. Uncertainty in mean values prohibits interpretation of mean *D. strigosa* Sr/Ca in terms of mean climate, but does not necessarily impact interannual or seasonal variations.

Table 7. Annual mean growth rates and Sr/Ca ratios with 1 σ standard error in modern corals.

	AN17	AN18	AN19
Number of years	18	28	10
Mean Sr/Ca (mmol/mol)	8.994 $\pm$ 0.004	9.129 $\pm$ 0.003	8.953 $\pm$ 0.005
Mean Extension rate (mm/year)	6.9 $\pm$ 0.4	5.6 $\pm$ 0.2	6.2 $\pm$ 0.4
Annual Sr/Ca-Extension correlation	0.16	0.32	0.14
p-value	0.55	0.10	0.71

4.2 Calibration

Calibration slopes obtained from Sr/Ca–SST regressions on the three modern corals using our four different methods (OLS, RMA, WLS and BWLS) are often statistically different from each other, but are mostly within a relatively narrow range of slopes compared to the range of Sr/Ca–SST slopes reported in the literature for a variety of species [Chen *et al.*, 2013; Corrège, 2006; DeLong *et al.*, 2011; Sadler *et al.*, 2014]. The fact that we obtained significantly different results with the same data indicates that a portion of the range of Sr/Ca–SST slopes in the literature can be attributed to different

466 regression techniques alone. Our analysis demonstrates that the assumptions about data
467 uncertainty inherent in each regression technique strongly impacts the resulting
468 regression slope obtained from any given data set. When the implicit assumptions about
469 data uncertainty do not reflect reality, the resulting slopes lead to biased estimations of
470 SST [*Solow and Huppert, 2004*].

471 Assessing temperature uncertainty has historically been very difficult for coral
472 calibration studies because our study sites are often remote and without long-term local
473 temperature monitoring. The recent release of ERSST v3b and HadSST gridded SST
474 data products which include gridbox-specific estimates of the mean monthly temperature
475 uncertainty provides at least some quantifiable uncertainty estimates when using gridded
476 SST data. This does not solve the fundamental issue of whether to calibrate with local
477 rather than gridded SST, but we point out that the coral is fundamentally experiencing
478 local SST, so calibrations using gridded data (present study included) will inherently
479 have some variance in Sr/Ca that is due to local SST and is not explainable with the
480 gridded SST data. Consequently, estimates of SST reconstruction error will be larger
481 than they might have been if accurate and precise local SST data were available.

482 Besides the choice of SST data to use, calibration studies need to choose a
483 regression technique. We recommend future calibration studies use the unbiased WLS
484 regression technique with either estimates of gridded SST uncertainty now available, or
485 estimates of local SST error based on an understanding of the local SST data and the
486 local coastal SST dynamics. The WLS calibration technique accounts for unequal errors
487 in both the dependent and independent variables and thus provides the best estimation of
488 the underlying Sr/Ca-SST relationship. MATLAB code available from [*Thirumalai et*

489 *al.*, 2011] makes implementation easily accessible to most researchers. Standardizing the
490 methods used for calibration may clarify if genus- or species-specific universal
491 calibrations as proposed by *Weber* [1973] are realistic or if ad-hoc calibrations at every
492 study site are necessary.

494 4.3 Towards a universal *Diploria strigosa* calibration

495 Accepting as a premise *Weber*'s [1973] assertion that a taxon-specific ideal
496 calibration exists, we combine Sr/Ca data from our study site with existing published
497 Sr/Ca from this species to quantify a best-possible Sr/Ca-SST relationship for *D. strigosa*:
498 $-0.0463(\pm 0.0004)$ mmol/mol/°C for mean-centered data (Figure 6), $-0.0590(\pm 0.0012)$
499 mmol/mol/°C for monthly anomalies and $-0.063 (\pm 0.004)$ for annual data. This result is
500 well within the range of results for the three Anegada corals. The five-coral result is
501 slightly steeper than the individual coral calibrations from Guadeloupe (0.042
502 mmol/mol/°C) [*Hetzinger et al.*, 2006] and Bonaire (0.034 mmol/mol/°C) [*Giry et al.*,
503 2012]. The use of five individual coral heads from three sites in the regression minimizes
504 the potential influence of differences between coral colonies to get a result that is more
505 appropriately applicable to an individual chosen from the population at random e.g., a
506 sub-fossil coral washed ashore. Future paleoclimate studies can use this calibration with
507 confidence that it is not a result skewed by the vagaries of a single colony or a single
508 study site.

509 Our combined regression is done with mean-centered, monthly anomaly, and
510 mean annual anomaly data separately to give other researchers the ability to choose
511 which they want to use because each has their benefits and drawbacks. All of the data

(monthly, monthly anomalies, and annual data) were set to zero mean before regression with temperature data to minimize any non-temperature related mean differences that might be due to differences in average growth rate, un-identified biological factors, or interlaboratory calibration issues. The mean-centered monthly data effectively calibrates the seasonal cycles of SST and Sr/Ca because the seasonal cycle dominates the variance of both records. Given the potential for within-year skeletal thickening and its potential impact on the apparent Sr/Ca-SST relationship [Gagan *et al.*, 2012], calibrations that include the seasonal cycle are most robust when applied to studies investigating the seasonal cycles of SST.

Ideally, calibrating with anomaly data is robust for investigating interannual and longer changes in SST. However, Sr/Ca-SST regression slopes obtained from anomaly data are not well characterized because of the low signal to noise ratios inherent in SST and coral Sr/Ca data and the sensitivity of the resulting regression slopes to methodological assumptions about data uncertainty. *DeLong et al.* [2014] point out that most of the scatter in a monthly anomaly Sr/Ca-SST regression is due to small sub-annual age-model errors, making monthly anomaly regressions inherently noisy and unreliable. Instead, annual average data provide the basis for our long-timescale calibration. Interestingly, with the Anegada corals, we get effectively the same Sr/Ca-SST relationship from the mean annual data as we do calibrating the seasonal cycle, implying that perhaps *Diploria strigosa* colonies do not thicken their skeletons throughout the tissue layer as Gagan *et al.* [2012] demonstrated for *Porites*. However, the five-coral multi-site calibration shows the expected increase in slope for the annual data regression, indicating that a more likely explanation for the Anegada-only results is that the smaller

number of data points and low signal to noise ratio make the true skeletal Sr/Ca-SST relationship difficult to precisely characterize.

Annual data have one major drawback similar to monthly anomalies: namely that there is less variance in SST, so you are calibrating over a very narrow range. The best thing to do to remedy this is a regional mean calibration with multiple corals, such as in the original *Weber* [1973] paper and more recently in *DeLong et al.* [2010]. However we could not conduct a similar regional mean calibration because the existing data for this species all come from reefs with the same long-term mean temperature. Additionally, the Sr/Ca data were produced in different labs that have not cross-calibrated and thus the data may have undetected instrument calibration issues [*Hawthorn et al.*, 2013].

5 Conclusions

In this study, we assess four different calibration regression methods and conclude that the standard practice of ordinary least squares regression should be replaced with weighted least squares regression given the typical distribution of error between the geochemistry and instrumental temperature data. Our calibration using *D. strigosa* from Anegada, British Virgin Islands is similar to previous calibrations using this species from other sites, suggesting that Sr/Ca-SST calibrations from our study are widely applicable to this species. We have produced a three-site, five-colony calibration that can be utilized for future paleoclimate reconstructions with *D. strigosa*. In addition, our results indicate that whereas significant mean differences among individuals at the study site were

observed, seasonal and interannual temperature variability can still be distinguished using the skeletal geochemistry of *D. strigosa*.

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References

- Budd, A. F., H. Fukami, N. D. Smith, and N. Knowlton (2012), Taxonomic classification of the reef coral family Mussidae (Cnidaria: Anthozoa: Scleractinia), *Zoological Journal of the Linnean Society*, 166(3), 465-529.
- Cardinal, D., B. Hamelin, E. Bard, and J. Pätzold (2001), Sr/Ca, U/Ca and $\delta^{18}\text{O}$ records in recent massive corals from Bermuda: relationships with sea surface temperature, *Chemical Geology*, 176(1-4), 213-233.
- Cavalli-Sforza, L. L., and A. W. Edwards (1967), Phylogenetic Analysis Models and Estimation Procedures, *American Journal of Human Genetics*, 19(3 Part 1), 233.
- Chen, T., K. Yu, and T. Chen (2013), Sr/Ca-sea surface temperature calibration in the coral *Porites lutea* from subtropical northern South China Sea, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 392, 98-104.
- Clarke, M. R. B. (1980), The reduced major axis of a bivariate sample, *Biometrika*, 67(2), 441-446.

- Cobb, K. M., C. D. Charles, H. Cheng, and R. L. Edwards (2003), El Nino/Southern Oscillation and tropical Pacific climate during the last millennium, *Nature*, 424(6946), 271-276.
- Cohen, A. L., and S. R. Thorrold (2007), Recovery of temperature records from slow-growing corals by fine scale sampling of skeletons, *Geophysical Research Letters*, 34(17).
- Cohen, A. L., S. R. Smith, M. S. McCartney, and J. van Etten (2004), How brain corals record climate: an integration of skeletal structure, growth and chemistry of *Diploria labyrinthiformis* from Bermuda, *Marine Ecology Progress Series*, 271, 147-158.
- Corrège, T. (2006), Sea surface temperature and salinity reconstruction from coral geochemical tracers, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 232(2-4), 408-428.
- Crowley, T. J., T. M. Quinn, and W. T. Hyde (1999), Validation of coral temperature calibrations, *Paleoceanography*, 14(5), 605-615.
- de Villiers, S., G. T. Shen, and B. K. Nelson (1994), The Sr/Ca-temperature relationship in coralline aragonite: Influence of variability in (Sr/Ca)seawater and skeletal growth parameters, *Geochimica et Cosmochimica Acta*, 58(1), 197-208.
- DeLong, K. L., J. A. Flannery, C. R. Maupin, R. Z. Poore, and T. M. Quinn (2011), A coral Sr/Ca calibration and replication study of two massive corals from the Gulf of Mexico, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 307(1-4), 117-128.
- DeLong, K. L., T. M. Quinn, and F. W. Taylor (2007), Reconstructing twentieth-century sea surface temperature variability in the southwest Pacific: A replication study using multiple coral Sr/Ca records from New Caledonia, *Paleoceanography*, 22(4), PA4212.
- DeLong, K. L., T. M. Quinn, C.-C. Shen, and K. Lin (2010), A snapshot of climate variability at Tahiti at 9.5 ka using a fossil coral from IODP Expedition 310, *Geochemistry, Geophysics, Geosystems*, 11(6), Q06005.
- DeLong, K. L., J. A. Flannery, R. Z. Poore, T. M. Quinn, C. R. Maupin, K. Lin, and C.-C. Shen (2014), A reconstruction of sea surface temperature variability in the southeastern Gulf of Mexico from 1734 to 2008 C.E. using cross-dated Sr/Ca records from the coral *Siderastrea siderea*, *Paleoceanography*, 29(5), 403-422.
- Draschba, S., J. Pätzold, and G. Wefer (2000), North Atlantic climate variability since AD 1350 recorded in $\delta^{18}\text{O}$ and skeletal density of Bermuda corals, *International Journal of Earth Sciences*, 88(4), 733-741.
- Efron, B. and R. Tibshirani (1986), Bootstrap methods for standard errors, confidence intervals and other measures of statistical accuracy, *Statistical Science*, 1(1), 54-75.
- Fitch, W. M., and E. Margoliash (1967), Construction of phylogenetic trees, *Science*, 155(760), 279-284.
- Gagan, M. K., G. B. Dunbar, and A. Suzuki (2012), The effect of skeletal mass accumulation in *Porites* on coral Sr/Ca and $\delta^{18}\text{O}$ paleothermometry, *Paleoceanography*, 27(1), PA1203.

- Giry, C., T. Felis, M. Kölling, and S. Scheffers (2010), Geochemistry and skeletal structure of *Diploria strigosa*, implications for coral-based climate reconstruction, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 298(3-4), 378-387.
- Giry, C., T. Felis, M. Kölling, D. Scholz, W. Wei, G. Lohmann, and S. Scheffers (2012), Mid-to late Holocene changes in tropical Atlantic temperature seasonality and interannual to multidecadal variability documented in southern Caribbean corals, *Earth and Planetary Science Letters*, 331, 187-200.
- Goodkin, N. F., K. A. Huguen, and A. L. Cohen (2007), A multicoral calibration method to approximate a universal equation relating Sr/Ca and growth rate to sea surface temperature, *Paleoceanography*, 22(1), PA1214.
- Goodkin, N. F., K. A. Huguen, A. L. Cohen, and S. R. Smith (2005), Record of Little Ice Age sea surface temperatures at Bermuda using a growth-dependent calibration of coral Sr/Ca, *Paleoceanography*, 20(4), PA4016.
- Hathorne, E. C., et al. (2013), Interlaboratory study for coral Sr/Ca and other element/Ca ratio measurements, *Geochemistry, Geophysics, Geosystems*, 14(9), 3730-3750.
- Hetzinger, S., M. Pfeiffer, W.-C. Dullo, D. Garbe-Schönberg, and J. Halfar (2010), Rapid 20th century warming in the Caribbean and impact of remote forcing on climate in the northern tropical Atlantic as recorded in a Guadeloupe coral, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 296(1-2), 111-124.
- Hetzinger, S., M. Pfeiffer, W.-C. Dullo, E. Ruprecht, and D. Garbe-Schönberg (2006), Sr/Ca and $\delta^{18}\text{O}$ in a fast-growing *Diploria strigosa* coral: Evaluation of a new climate archive for the tropical Atlantic, *Geochemistry, Geophysics, Geosystems*, 7(10), Q10002.
- Kilbourne, K. H., T. M. Quinn, R. Webb, T. Guilderson, J. Nyberg, and A. Winter (2008), Paleoclimate proxy perspective on Caribbean climate since the year 1751: Evidence of cooler temperatures and multidecadal variability, *Paleoceanography*, 23(3), PA3220.
- Kuhnert, H., J. Pätzold, B. Schnetger, and G. Wefer (2002), Sea-surface temperature variability in the 16th century at Bermuda inferred from coral records1, *Palaeogeography, Palaeoclimatology, Palaeoecology*, 179(3-4), 159-171.
- McGregor, H. V., and M. K. Gagan (2003), Diagenesis and geochemistry of *Porites* corals from Papua New Guinea: Implications for paleoclimate reconstruction, *Geochimica et Cosmochimica Acta*, 67(12), 2147-2156.
- Nurhati, I. S., K. M. Cobb, C. D. Charles, and R. B. Dunbar (2009), Late 20th century warming and freshening in the central tropical Pacific, *Geophysical Research Letters*, 36(21), L21606.
- Paillard, D., L. Labeyrie, and P. Yiou (1996), Macintosh Program performs time-series analysis, *Eos, Transactions American Geophysical Union*, 77(39), 379-379.
- Pfeiffer, M., W.-C. Dullo, J. Zinke, and D. Garbe-Schönberg (2008), Three monthly coral Sr/Ca records from the Chagos Archipelago covering the period of 1950–1995 A.D.: reproducibility and implications for quantitative reconstructions of sea surface temperature variations, *International Journal of Earth Sciences*, 98(1), 53-66.
- Quinn, T. M., and D. E. Sampson (2002), A multiproxy approach to reconstructing sea surface conditions using coral skeleton geochemistry, *Paleoceanography*, 17(4), 1062.

- Reynolds, R. W., T. M. Smith, C. Liu, D. B. Chelton, K. S. Casey, and M. G. Schlax (2007), Daily high-resolution-blended analyses for sea surface temperature, *Journal of Climate*, 20(22), 5473-5496.
- Sadler, J., G. E. Webb, L. D. Nothdurft, and B. Dechnik (2014), Geochemistry-based coral palaeoclimate studies and the potential of 'non-traditional' (non-massive Porites) corals: Recent developments and future progression, *Earth-Science Reviews*, 139, 291-316.
- Saenger, C., A. L. Cohen, D. W. Oppo, and D. Hubbard (2008), Interpreting sea surface temperature from strontium/calcium ratios in *Montastrea* corals: Link with growth rate and implications for proxy reconstructions, *Paleoceanography*, 23(3), PA3102.
- Schrag, D. P. (1999), Rapid analysis of high-precision Sr/Ca ratios in corals and other marine carbonates, *Paleoceanography*, 14(2), 97-102.
- Shen, C.-C., H. Cheng, R. L. Edwards, S. B. Moran, H. N. Edmonds, J. A. Hoff, and R. B. Thomas (2003), Measurement of attogram quantities of ^{231}Pa in dissolved and particulate fractions of seawater by isotope dilution thermal ionization mass spectroscopy, *Analytical Chemistry*, 75(5), 1075-1079.
- Shen, C.-C., T. Lee, C.-Y. Chen, C.-H. Wang, C.-F. Dai, and L.-A. Li (1996), The calibration of $D[\text{Sr}/\text{Ca}]$ versus sea surface temperature relationship for *Porites* corals, *Geochimica et Cosmochimica Acta*, 60(20), 3849-3858.
- Shen, C.-C., C.-C. Wu, H. Cheng, R. Lawrence Edwards, Y.-T. Hsieh, S. Gallet, C.-C. Chang, T.-Y. Li, D. D. Lam, and A. Kano (2012), High-precision and high-resolution carbonate ^{230}Th dating by MC-ICP-MS with SEM protocols, *Geochimica et Cosmochimica Acta*, 99, 71-86.
- Shen, C.-C., et al. (2008), Variation of initial $^{230}\text{Th}/^{232}\text{Th}$ and limits of high precision U-Th dating of shallow-water corals, *Geochimica et Cosmochimica Acta*, 72(17), 4201-4223.
- Smith, R. J. (2009), Use and misuse of the reduced major axis for line - fitting, *American Journal of Physical Anthropology*, 140(3), 476-486.
- Smith, T. M., and R. W. Reynolds (2004), Improved extended reconstruction of SST (1854-1997), *Journal of Climate*, 17(12), 2466-2477.
- Smith, T. M., R. W. Reynolds, T. C. Peterson, and J. Lawrimore (2008), Improvements to NOAA's historical merged land-ocean surface temperature analysis (1880-2006), *Journal of Climate*, 21(10), 2283-2296.
- Smith, J. M., T. M. Quinn, K. P. Helmle, and R. B. Halley (2006), Reproducibility of geochemical and climatic signals in the Atlantic coral *Montastraea faveolata*, *Paleoceanography*, 21(1), PA1010.
- Solow, A. R., and A. Huppert (2004), A potential bias in coral reconstruction of sea surface temperature, *Geophysical Research Letters*, 31(6), L06308.
- Stephans, C. L., T. M. Quinn, F. W. Taylor, and T. Corrège (2004), Assessing the reproducibility of coral - based climate records, *Geophysical Research Letters*, 31(18).
- Swart, P. K., H. Elderfield, and M. J. Greaves (2002), A high-resolution calibration of Sr/Ca thermometry using the Caribbean coral *Montastraea annularis*, *Geochemistry, Geophysics, Geosystems*, 3(11), 8402.

719 Thirumalai, K., A. Singh, and R. Ramesh (2011), A MATLAB™ code to perform
 720 weighted linear regression with (correlated or uncorrelated) errors in bivariate
 721 data, *Journal of the Geological Society of India*, 77(4), 377-380.
 722 Watanabe, T., A. Winter, and T. Oba (2001), Seasonal changes in sea surface temperature
 723 and salinity during the Little Ice Age in the Caribbean Sea deduced from Mg/Ca
 724 and $^{18}\text{O}/^{16}\text{O}$ ratios in corals, *Marine Geology*, 173(1-4), 21-35.
 725 Watanabe, T., A. Winter, T. Oba, R. Anzai, and H. Ishioroshi (2002), Evaluation of the
 726 fidelity of isotope records as an environmental proxy in the coral *Montastraea*,
 727 *Coral Reefs*, 21(2), 169-178.
 728 Weber, J. N. (1973), Incorporation of strontium into reef coral skeletal carbonate,
 729 *Geochimica et Cosmochimica Acta*, 37(9), 2173-2190.
 730 York, D., N. M. Evensen, M. L. Martinez, and J. D. B. Delgado (2004), Unified
 731 equations for the slope, intercept, and standard errors of the best straight line,
 732 *American Journal of Physics*, 72(3), 367-375.
 733