Supplementary TextS1: Bayesian Calculation

To take the uncertainty in the calibration of Mg/Ca to SST into account, the error in the calibration must be known. The form of the Mg/Ca-based temperature calibration is exponential:

$$Mg/Ca=Be^{AT}$$

where T is temperature in °C and A is the sensitivity to temperature. Numerous calibrations for the planktonic foraminifer *Globigerinoides ruber* have been proposed, and are based on samples obtained from culturing study [*Kisakürek et al.*, 2008], sediment trap [*Anand et al.*, 2003; *McConnell and Thunell*, 2005], and core top material [*Dekens et al.*, 2002]. For uncertainty quantification using the Bayesian approach, culturing studies present the advantage that the independent variable (in this case temperature) is precisely known. This motivates our choice of using the *Kisakürek et al.* [2008] dataset to develop a calibration equation for use in this study.

Here, we develop the calibration equation using the Bayesian approach, which allows us the obtain all the possible solutions of the coefficients A and B, and compare the results to the more traditionally used least-square procedure. Bayesian statistics employs algorithms to draw a set of samples from prior probability distributions and update the probability of the set of parameters in light of the current data [*Bolstad*, 2010]. The characteristics of the prior distribution is determined by information available before the current data has been analyzed, and can even reflect the analyst's subjective judgement about the parameter [*Wilks*, 2011]. Bayes' theorem then combines the prior density distribution and the current data in the posterior probability distribution of the parameter, which measures how plausible the prior value of the parameter is after we have observed the data [*Bolstad*, 2010].

1. Least-Square Regression

A nonlinear least-square regression between the *G. ruber* Mg/Ca and temperature leads to the following equation (95% confidence level included in parenthesis):

$$Mg/Ca=0.45(\pm0.3)e^{0.09(\pm0.02)T}$$

A plot of the measured values with the least-square solution and its 95% confidence interval is provided in Figure S1a. It should be noted that randomly drawing a new values for the pre-exponential and exponential coefficients from a Gaussian distribution [*Marcott et al.*, 2013] does not necessarily provide valid equations that could represent the data since in a regression, the A and B coefficients are correlated.

2. Bayesian Approach

We used uniform distributions as prior distributions for the A and B coefficients. The [min,max] values were set at [0.05, 0.15] for A and [0.2, 0.8] for B. The Bayesian calculation enables us to

enumerate sets of the unknown coefficients that allow the observational temperature to a fit a model of Mg/Ca measurements to within the analytical precision. And it does this through a Markov Chain Monte Carlo (MCMC) that includes random sampling and a transition probability that is related to the error in any one model fit. The frequency of the sample selected provides an estimate of the joint probability for the parameters considered. The joint probability for each parameter can be visualized by constructing a histogram of how often each parameter was selected. In this study, we used the Metropolis-Hastings algorithm [*Hastings*, 1970]. The basic idea behind this algorithm is to use a random walk on the proposed density distribution to generate a series of samples that are linked in a Markov Chain (i.e., each sample is correlated only directly to the previous one) and a method for rejecting or accepting the proposed moves:

- Step 1: Values for the regression coefficients were randomly drawn from the prior distributions.
- Step 2: The cost function ($cost_1$) was then calculated as:

$$\text{cost} = \frac{\sum\left(\left(Mg/Ca\right)_{\text{modeled}} - \left(Mg/Ca\right)_{\text{measured}}\right)^2}{2\sigma}$$

where the modeled Mg/Ca is obtained from the regression equation, the measured Mg/Ca is the observed foraminiferal Mg/Ca value, σ is the ±1σ error on the Mg/Ca estimate (±0.15mmol/mol [*Kisakürek et al.*, 2008].

- Step 3: Step from the current position in parameter space to a new point and a new cost ($cost_2$) is calculated. The ideal step size is problem specific, which mainly determines convergence rates rather than the result of the calculation.
- Step 4: If $cost_1 > cost_2$, the new coefficients were accepted and these new coefficients were then used as the basis for the next iteration. If $cost_2 > cost_1$, the new parameters were then accepted with probability $p=\exp(cost_1-cost_2)$. That is, a random sample r was drawn from a uniform distribution with [min,max]=[0,1]. If p>r, these new parameters would be accepted and used as the point to step from for the next iteration. Else, the new parameters would be rejected and the previously-accepted parameters would be used as the starting point for the next iteration. This process is repeated 50,000 times. The final distribution neglects the first 1000 trials (Figure S1c,d).

For the purpose of this study, we randomly selected 10,000 of these models for used in uncertainty quantification.

We used a similar process to generate possible solutions to the *Bemis et al.* [1998] equation to estimate the uncertainty in the $\delta^{18}O_{sw}$ record. In this case, the model takes the form:

$$\delta_c - \delta_w = aT + b$$

The prior distributions for the a and b coefficients were also set as uniform distributions with [min,max] values of [-0.25, -0.15] and [2.5 3.5] respectively. The error estimate on the δ_c-δ_w is estimated as the combined error on the δ_c and δ_w measurements as $\sqrt{0.05^2 + 0.03^2}$.

3. Comparison to least-square solution

The solution set that minimizes the cost function is equivalent to the least-square solution derived previously (Figure S1a). This results is not surprising since the minimum cost represents the solution that minimizes the residuals between the model and the data. However, plotting the solution sets that fall within the lower 95% of the cost does not fill the 95% confidence interval for the least square solution.

This discrepancy is due to the small sample size used to derive the least-square solution, which is based on minimizing the residuals. For a large number of datapoints, the sum of the residuals, expressed as the root mean square error (RMSE) would approximate the error in the data (in this case the analytical uncertainty). However, with only 5 data points, the residuals are not a good approximation of the analytical uncertainty.

The correlation between the A and B coefficients estimated from the Bayesian calculation is -0.99 ($p<0.01$), highlighting the fact that randomly selecting coefficients from their error envelope in not appropriate.

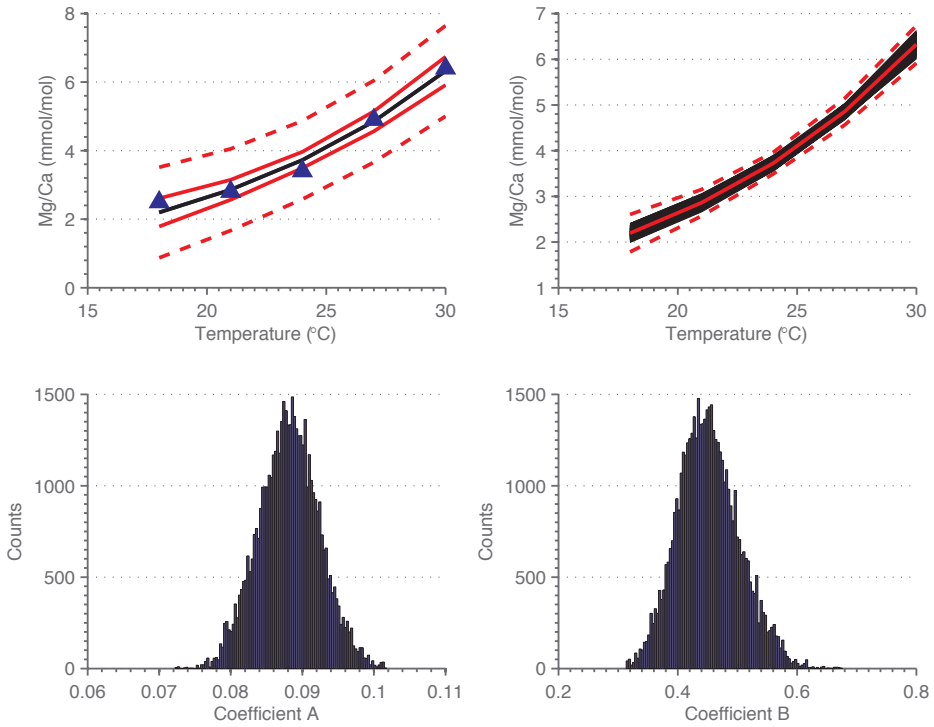

Figure S1: a. Measured Mg/Ca vs temperature (triangles) obtained from the temperature-only experiment of *Kisakürek et al.* [2008]. The red solid line represents the 95% confidence interval of the fit while the dashed line represents the 95% prediction interval. The black solid line represents the Bayesian solution that minimizes the cost function, which is equivalent to the least square solution. **b.** The red solid line represents the least-square solution while the red dashed line corresponds to the 95% confidence interval of the least-square solution. The black lines represent the 95% lowest cost of the Bayesian solutions. **c**. Histograms of possible values for coefficient A. **d.** Same as **c.** for coefficient B.

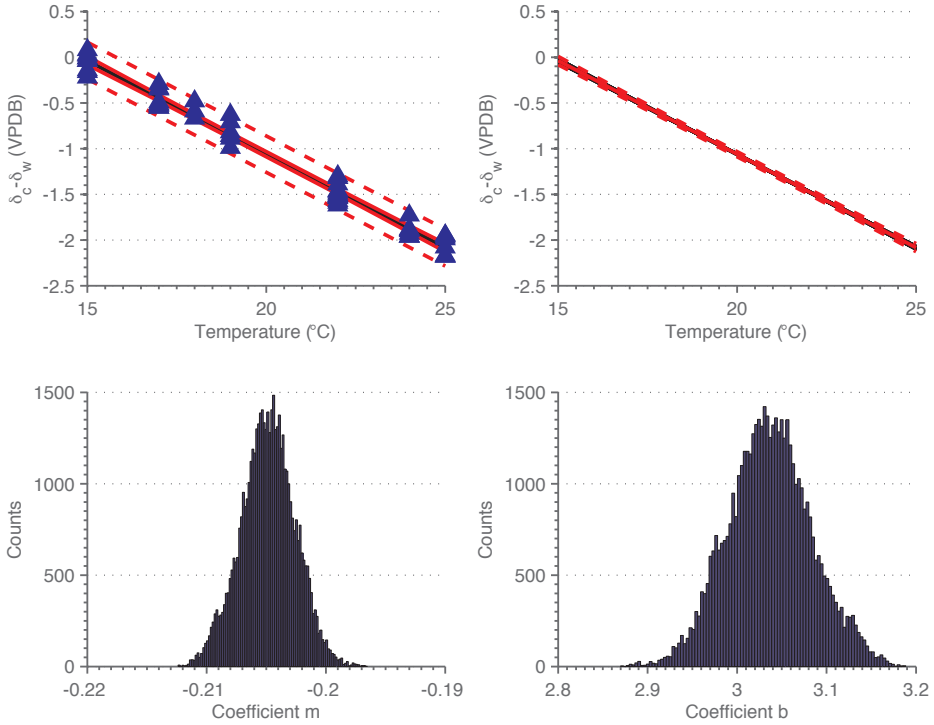

Figure S2: a. Measured δ_c-δ_w vs temperature (triangles) obtained from the *Bemis et al.* [1998] culturing study. The red solid line represents the 95% confidence interval of the fit while the dashed line represents the 95% prediction interval. The black solid line represents the Bayesian solution that minimizes the cost function, which is equivalent to the least square solution. **b.** The red solid line represents the least-square solution while the red dashed line corresponds to the 95% confidence interval of the least-square solution. The black lines represent the 95% lowest cost of the Bayesian solutions. **c**. Histograms of possible values for coefficient A. **d.** Same as **c.** for coefficient b.

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