

# Reconstructing seawater $\delta^{18}\text{O}$ from paired coral $\delta^{18}\text{O}$ and Sr/Ca ratios: Methods, error analysis and problems, with examples from Tahiti (French Polynesia) and Timor (Indonesia)

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## Abstract

We compare several statistical routines that may be used to calculate  $\delta^{18}\text{O}_{\text{sw}}$  and SSS from paired coral Sr/Ca and  $\delta^{18}\text{O}$  measurements. Typically, the  $\delta^{18}\text{O}_{\text{coral}}$ –SST relationship is estimated by linear regression of coral  $\delta^{18}\text{O}$  vs. SST. If this method is applied, evidence should be given that at a particular site SST and SSS do not co-vary. In the tropical oceans, SST and  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) often co-vary, and this will bias the estimate of the regression slope of  $\delta^{18}\text{O}_{\text{coral}}$ –SST. Using a stochastic model, we show that covariance leads to a bias in the coefficients of the univariate regression equations. As the slope of the  $\delta^{18}\text{O}_{\text{coral}}$ –SST relationship has known, we propose to insert this value for  $\gamma_1$  in the regression models. This requires that the constants of the regression equations are removed. To omit the constants, we propose to center the regression equations (i.e., to remove the mean values from the variables). The statistical error propagation is calculated to assess our ability to resolve past variations in  $\delta^{18}\text{O}_{\text{sw}}$  (SSS). At Tahiti, we find that the combined analytical uncertainties of coral  $\delta^{18}\text{O}$  and Sr/Ca equal the amplitude of the seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS). Therefore, we cannot resolve the seasonal cycle of SSS at Tahiti. At Timor, the error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) is lower than the magnitude of seasonal variations of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS), and the seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) can be resolved.

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## 1. INTRODUCTION

The oxygen isotopic composition of seawater ( $\delta^{18}\text{O}_{\text{sw}}$ ) is related to the hydrological balance [precipitation–evaporation (P–E)] and, by extension, to sea surface salinity (SSS)

(e.g., Craig and Gordon, 1965; Schmidt, 1999; Delaygue et al., 2000). Both are important climatic parameters. Therefore, reconstructing  $\delta^{18}\text{O}_{\text{sw}}$  is an important aspect of coral paleoclimatology. The main objective of coral-based  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions is to reconstruct past variations of SSS on time scales ranging from seasonal to centennial (e.g., Hendy et al., 2002; Ren et al., 2002).

The  $\delta^{18}\text{O}$  composition of scleractinian corals is influenced by both sea surface temperature (SST) and seawater  $\delta^{18}\text{O}$  ( $\delta^{18}\text{O}_{\text{sw}}$ ) (Ren et al., 2002; Corregge et al., 2004; Pfeiffer et al., 2004; Pfeiffer et al., 2006). In contrast, several studies have confirmed that Sr/Ca is a reliable proxy for SST (Beck et al., 1992; McCulloch et al., 1994; Shen et al., 1996; Alibert and McCulloch, 1997; Marshall and McCulloch,

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2002; Pfeiffer et al., 2006), provided that calcification and growth-related effects are minimized by sampling the coral along its main growth axis (McCulloch et al., 1994; Alibert and McCulloch, 1997; Marshall and McCulloch, 2002). Therefore, paired coral  $\delta^{18}\text{O}$  and Sr/Ca measurements can be used to reconstruct  $\delta^{18}\text{O}_{\text{sw}}$ . The statistical methods that should be used for  $\delta^{18}\text{O}_{\text{sw}}$  calculations, however, have been a matter of intense debate over the past few years (Gagan et al., 1998; Ren et al., 2002; Huppert and Solow, 2004; Kilbourne et al., 2004). While interannual to decadal  $\delta^{18}\text{O}_{\text{sw}}$  variations inferred from corals have been linked successfully to instrumental data of sea surface salinity, the reconstruction of seasonal-scale  $\delta^{18}\text{O}_{\text{sw}}$ /SSS variations appears problematic due to the noisiness of the coral proxy data (e.g., Kilbourne et al., 2004).

The most commonly accepted oxygen isotope paleotemperature scale in use today for biogenic carbonates is that proposed by Grossman and Ku (1986) and has the format  $T = m*(\delta^{18}\text{O} - \delta^{18}\text{O}_{\text{sw}}) + b$ . McCulloch et al. (1994) and Gagan et al. (1998) first demonstrated that  $\delta^{18}\text{O}_{\text{sw}}$  can be reconstructed from paired coral  $\delta^{18}\text{O}$  and Sr/Ca measurements. The authors estimate the relationship of coral  $\delta^{18}\text{O}$  and SST, as well as Sr/Ca and SST, using univariate linear regression equations. These equations are then used to convert both proxies to temperature units, in order to subtract the temperature component from coral  $\delta^{18}\text{O}$ . Because the absolute values of coral  $\delta^{18}\text{O}$  and Sr/Ca are not considered reliable (e.g., Linsley et al., 1999; Suzuki et al., 2005), Ren et al. (2002), proposed to omit the intercept values of the  $\delta^{18}\text{O}_{\text{coral}}$  (Sr/Ca)–SST regression by calculating the first derivatives of the two proxies. Previous studies compared the two methods and found that the results obtained are identical provided that the same slope parameters are used (e.g., Huppert and Solow, 2004; Kilbourne et al., 2004). Huppert and Solow (2004) realized that changes in  $\delta^{18}\text{O}_{\text{sw}}$  are a potential problem for  $\delta^{18}\text{O}_{\text{sw}}$ /SSS reconstructions from corals, as these may bias the coral  $\delta^{18}\text{O}$ –SST slope in the univariate  $\delta^{18}\text{O}_{\text{coral}}$ –SST regression, and this biased parameter is then used to reconstruct  $\delta^{18}\text{O}_{\text{sw}}$ . However, the authors simply state that ‘this possibility poses the same problem to both [ANU and Ren et al., 2002] methods’.

As we will show in this paper, covariant changes in SST and  $\delta^{18}\text{O}_{\text{sw}}$  will bias the regression slope of the  $\delta^{18}\text{O}_{\text{coral}}$ –SST relationship if  $\delta^{18}\text{O}_{\text{coral}}$  is calibrated with SST only. Therefore,  $\delta^{18}\text{O}_{\text{sw}}$  calculations using univariate  $\delta^{18}\text{O}_{\text{coral}}$ –SST regression models, as proposed by McCulloch et al. (1994) and Gagan et al. (1998) are problematic. We will use new paired coral  $\delta^{18}\text{O}$  and Sr/Ca records from Tahiti (French Polynesia) and Timor (Indonesia) (Fig. 1), each covering 20 years, as well as simulated proxy data to illustrate this problem. Furthermore, we will compare and discuss the methods proposed for  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions from corals, and suggest using a simpler, well established statistical method to omit the intercept values from the  $\delta^{18}\text{O}$  (Sr/Ca)–SST regression equation. We also explore how SST covariant changes in  $\delta^{18}\text{O}_{\text{sw}}$  and SSS would affect coral-based reconstructions and how we could avoid this potential problem in the future. For all approaches, the error propagation of calculated  $\delta^{18}\text{O}_{\text{sw}}$  is discussed. Since

$\delta^{18}\text{O}_{\text{sw}}$  is related to SSS, our  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions are compared with SSS data from the Simple Ocean Data Assimilation (SODA) model (Carton et al., 2000).

## 2. CLIMATIC AND OCEANOGRAPHIC SETTING OF THE STUDY AREAS

### 2.1. Tahiti, French Polynesia

Tahiti (149°20'W 17°4'S) is located in the Southwestern tropical Pacific (24°S–10°S; 160°E–140°W) (Fig. 1). This region is characterized by a major salinity front that separates the high salinity waters formed in the subtropical region (120°W, 20°S), where evaporation exceeds precipitation, from the low salinity waters formed in the warm pool area, where precipitation exceeds evaporation (Gouriou and Delcroix, 2002). Fig. 2a compares climatological data of SST and SSS at Tahiti from SODA v. 1.4.2. Both SST and SSS show a clear seasonal cycle. SST ranges from 26.3 °C in August to 28.8 °C in March. SSS ranges from 35.7 psu in April to 36.1 psu in October. SST and SSS co-vary, but are out of phase. Maximum (minimum) SSS lags minimum (maximum) SST by 1–2 month.

Interannual salinity and SST variations in the Southwestern tropical Pacific are linked to ENSO (Gouriou and Delcroix, 2002; Ouilion et al., 2005). Thus, SST covariant changes in SSS (and  $\delta^{18}\text{O}_{\text{sw}}$ ) occur on seasonal and interannual time scales.

### 2.2. Timor, Indonesia

The Indonesian region experiences a wet season during the Northwest (NW) monsoon (December–March), when the northeasterly winds blow from the north across the equator. SST in Indonesia then ranges between ~28.5 and 30 °C. The northeasterly winds push low salinity water from the South China Sea into the Makassar Strait, a main passage of the Indonesian Throughflow (ITF). During the South East (SE) monsoon (June–September), when prevailing southeast winds blow from Australia, SST ranges between ~26 and 29 °C and low salinity waters are found further to the east in the Banda sea (Gordon et al., 2004). The Timor coral site is located in Ombai strait (123°3E, 10°1S), which is one of the main ITF exit passages (Fig. 1). Therefore, SST and SSS can be influenced both by oceanic advection and atmospheric phenomena (e.g., monsoonal processes).

Fig. 2b compares climatological data of SST and SSS at Timor. Both SST and SSS show a clear seasonal cycle. SST ranges from 26.8 °C in August to 30 °C in December. SSS ranges from 34 psu in July to 34.4 psu in January. At Timor, SST and SSS co-vary in phase. Maximum (minimum) SSS coincides with maximum (minimum) SST.

## 3. MATERIALS AND METHODS

In July 1995, we drilled two coral cores from massive colonies of *Porites* sp. growing in the lagoon of Tahiti (French Polynesia). Core TH1 was taken at Teahupoo, in the south-eastern part of the lagoon. Core TH2 was drilled

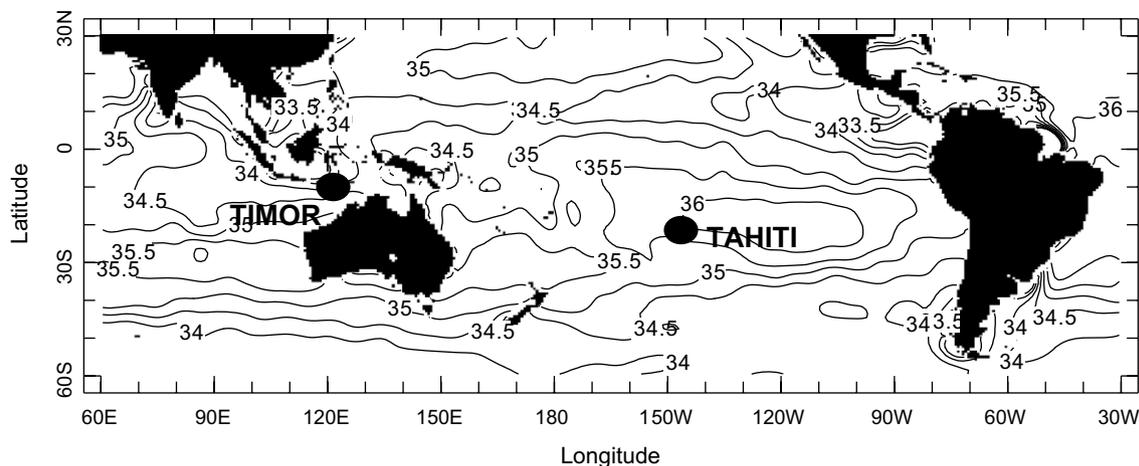


Fig. 1. Map showing the mean surface salinity in January–March (contours) and coral drilling sites of Timor and Tahiti (black circles).

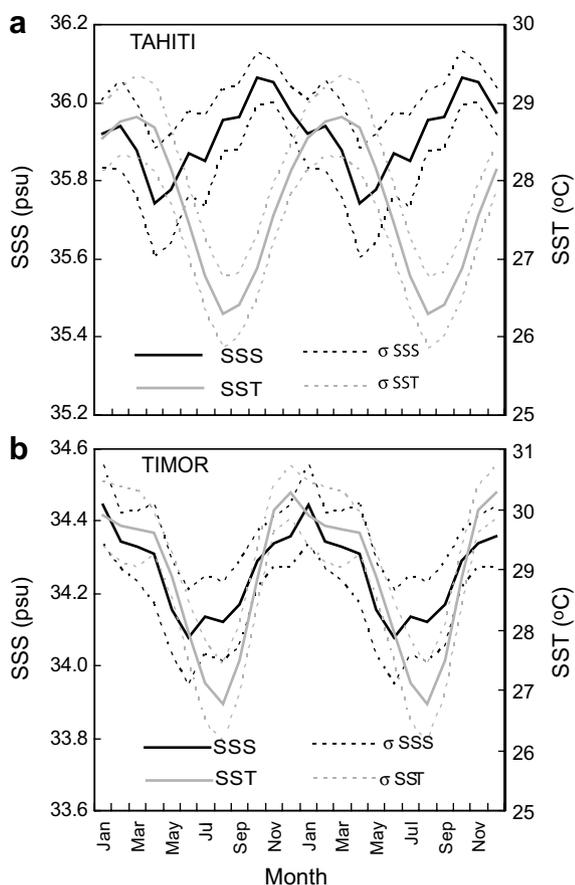


Fig. 2. Monthly mean SSS (solid black lines) and SST (solid gray lines) for (a) Tahiti and (b) Timor. The climatology is calculated over the time period of 1958–1995 (Tahiti) and 1958–2004 (Timor). Dashed lines: standard deviation ( $1\sigma$ ) of monthly mean SSS (black) and SST data (gray). SSS and SST are obtained from SODA v. 1.4.2. Note that at both sites, SST and SSS co-vary: at Timor, SSS and SST co-vary in phase while at Tahiti SSS and SST co-vary out of phase.

at Vairao. At Timor (Indonesia), a third core (KP1) was drilled in June 2004.

The X-radiographs of the slabs show annual density bands that allow a precise chronology. The average annual linear extension rate is approximately  $2 \pm 0.5$  cm/year. A sampling transect that follows the main growth axis was chosen. Slabs were subsampled with a dental drill using a drilling bit of 1 mm. Powdered samples were taken every 1 mm to get monthly resolved proxy records. The powdered samples were split for stable oxygen isotope ( $\delta^{18}\text{O}$ ) and trace element (Sr/Ca ratios) analysis.

We measured Sr/Ca ratios on a Spectro Ciros CCD SOP Inductively Coupled Plasma Optical Emission Spectrophotometer (ICP-OES) at the University of Kiel following a combination of the techniques described by Schrag (1999) and de Villiers et al. (2002). The sample solution is prepared by dissolving approximately 0.5 mg of coral powder in 1.00 mL  $\text{HNO}_3$  70%. The working solution is prepared by serial dilution of the sample solution with  $\text{HNO}_3$  2% to get a concentration of ca. 8 ppm Ca. Standard solution is prepared by dilution of 1.00 mL of the stock solution (0.52 g of coral powder from an in-house standard in 250 mL  $\text{HNO}_3$  2%) with 2.00 mL  $\text{HNO}_3$  2%. Sr and Ca lines, which are used for this measurement, are 407 and 317 nm, respectively. Analytical precision on Sr/Ca determinations is 0.15% RSD or 0.01 mmol/mol ( $1\sigma$ ) (based on replicate measurements,  $n = 74$ ).

The stable oxygen isotopic composition ( $\delta^{18}\text{O}$ ) was analyzed at IFM-GEOMAR. Core TH1 was analyzed using a Finnigan Mat 251 mass spectrometer. A Thermo Finnigan Gasbench II Delta Plus was used for the analysis of core TH2 and KP1. The isotope ratios are reported in ‰ notation relative to VPDB using NBS 19 as standard reference material. The analytical uncertainty is less than 0.06‰ ( $1\sigma$ ) for  $\delta^{18}\text{O}$  measurements, based on multiple measurements of an in-house carbonate standard (13 standards per 48 samples), which was calibrated against NBS-19.

The chronologies of TH1, TH2 and KP1 were constructed by linear interpolation between anchor points that were tied to the seasonal minima (maxima) of the Sr/Ca records. The same anchor points were used for the interpolation of the  $\delta^{18}\text{O}$  records. It is assumed that the minimum (maximum) skeletal Sr/Ca corresponds to the maximum

(minimum) SST. At Tahiti, the seasonal mean maximum (minimum) Sr/Ca is tied to August (March), which is on average the coolest (warmest) month. At Timor, the seasonal maximum (minimum) of Sr/Ca is tied to August (December). The uncertainty of the age model is approximately 2 months in any given year. At Tahiti, we use the average proxy record computed from TH1 and TH2. The proxy data is converted to time prior to averaging. Averaging should reduce the noisiness of the proxy records. We only use the data of the most recent 20 years (1975–1995). At Timor, only one single proxy record is available from the core top of KP1. Again, we only use the most recent 20 years of the Timor core (1985–2004) (Fig. 3).

#### 4. SALINITY DATA

##### 4.1. The SODA data

The Simple Ocean Data Assimilation (SODA) reanalysis project, which began in the mid 1990s, is an ongoing effort to reconstruct historical ocean climate variability on space and time scales similar to those captured by the atmospheric reanalysis projects (e.g., Carton et al., 2000). SODA provides monthly averages of SST and SSS data extending back until 1950. The data is mapped onto a uniform  $0.5^\circ \times 0.5^\circ$  grid (Carton et al., 2000). The SODA model uses input data from the World Ocean Database 2001, hydrographic data, satellite and in situ SST and altimetry from Geosat, ERS-1 and TOPEX/Poseidon (Carton et al., 2000). The last date of instrumental salinity measurements in 1990, and also the lack of satellite altimetry before 1986 constrain the quality of SODA data. However, at present SODA provides the most sophisticated global-scale salinity product. We use SODA version 1.4.2 which extends from 1958 to 2001. SODA 1.4.2 uses the surface wind products from ECMWF ERA 40. This product requires correction of the mean stress, which may be problematic in the tropics (Carton et al., 2000). The latest version of SODA is version 1.4.3., which uses daily wind data from the QuikSCAT scatterometer to overcome possible wind errors in the tropics. Unfortunately, SODA v. 1.4.3 only extends from 2000 to 2004. At Timor, we therefore combined SSS from SODA 1.4.2 and 1.4.3 for a comparison with the coral proxies.

##### 4.1.1. Historical salinity data and SODA

Instrumental records of past salinity variations are scarce. At Tahiti, several instrumental salinity (SSS) datasets are available. Delcroix et al. (1996) and Gouriou and Delcroix (2002) (hereafter referred to as SSS Delcroix) published monthly salinity data for the Southwestern tropical Pacific from ship-of-opportunity measurements. The dataset extends back until 1976 and is averaged over  $2^\circ$  latitude  $\times$   $10^\circ$  longitude. Local salinity measurements were made at Papeete, Tahiti (Fig. 4a) and are available from *L'Institut français de Recherche scientifique pour le Développement en coopération* (IRD) (Boiseau et al., 1998) (hereafter referred to as SSS IRD). SSS IRD covers 11 years and extends from 1979 until 1990. Unfortunately, this is too short for proxy calibration ( $n = 11$  for annual mean calibrations).

Fig. 4b compares monthly variations of instrumental surface salinity data measured at Tahiti (SSS Delcroix and SSS IRD) with SSS from SODA. The mean seasonal cycle of SSS SODA is similar with SSS IRD, which was measured at Papeete between 1979 and 1990 (see Figs. 4b and c). The correlation between both time series is high ( $R = 0.71$ ). SSS SODA correctly captures the seasonal cycle of SSS at Tahiti, but it may underestimate the magnitude of interannual-scale variability.

At Timor, SSS was measured by Sprintall et al. (2003) at two sites in Ombai strait, Ombai (northern Timor) and Roti (southern Timor) (hereafter referred to as SSS Ombai and SSS Roti, respectively) (Fig. 4a). The correlation between SSS Ombai (Location 2, Fig. 4a) and SSS Roti (Location 3, Fig. 4a) is high in the period of overlap ( $R = 0.61$ ). Unfortunately, the longest continuously available time series of SSS at Timor only extends from 1996 to 1998 (Fig. 4d) (Sprintall et al., 2003). For Timor, we extracted surface salinity data from SODA in the grid centered at  $10^\circ 12' S$ ,  $123^\circ 31' E$ . The correlation between SSS SODA and SSS Roti (SSS Ombai) is  $R = 0.77$  ( $R = 0.37$ ). The phase of the seasonal salinity cycle in SODA matches the instrumental data well (Fig. 4d), although we note that the amplitude of the seasonal cycle in SODA is somewhat lower than measured at Roti and Ombai.

Fig. 4e compares the mean seasonal cycle of SSS SODA with climatological salinity data from Levitus et al. (1994) (hereafter referred to as SSS Levitus). The seasonal amplitude of SSS Levitus is also larger than the amplitude of SSS SODA (Fig. 4e). We conclude that SSS SODA captures the phase of the seasonal salinity cycle reasonably well, although the magnitude of seasonal-scale salinity variations could be underestimated in the dataset (note: there is no indication that seasonal-scale SSS variations are overestimated in SODA).

In this study, we decided to use SSS SODA rather than instrumental salinity datasets, despite the potential problems of SODA indicated in Fig. 4. Only the SODA data is available at both Tahiti and Timor. Furthermore, a strong focus of this paper will be on the reconstruction of seasonal-scale SSS variations and the limitations imposed by the amplitude of the seasonal cycle and the analytical error. At Tahiti and Timor SSS SODA correctly captures the phase of the seasonal salinity cycle (at Timor, it may underestimate its magnitude). However, other gridded product of SSS may have similar biases, but the sparseness of local SSS measurement make an objective selection of the best SSS product very difficult. We therefore concentrate on the SODA SSS data.

## 5. THE RECONSTRUCTION OF $\Delta^{18}\text{O}$ SEAWATER: METHODOLOGIES

### 5.1. McCulloch et al. (1994), Gagan et al. (1998) and Ren et al. (2002)

The most commonly used technique to calculate  $\delta^{18}\text{O}_{\text{sw}}$  from paired coral  $\delta^{18}\text{O}$  and Sr/Ca measurements is to estimate the linear regression equations of coral  $\delta^{18}\text{O}$ –SST, as well as coral Sr/Ca–SST, using the simpli-

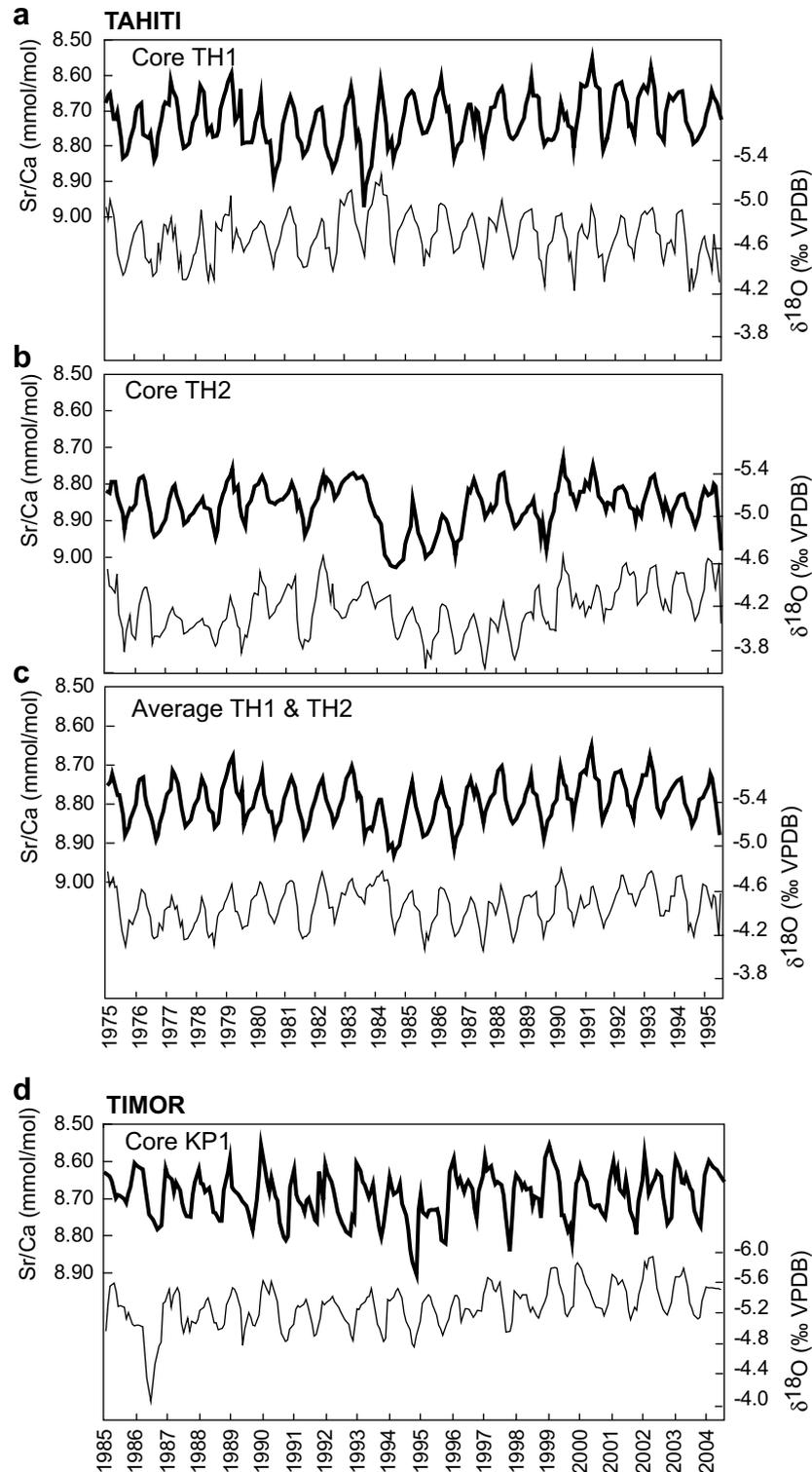


Fig. 3. Monthly coral  $\delta^{18}\text{O}$  (thin lines) and Sr/Ca (bold lines) records for the time period of 1975–1995 from Tahiti: (a) TH1 (b) TH2, (c) average proxy record of TH1 and TH2. (d) Monthly coral  $\delta^{18}\text{O}$  (thin line) and Sr/Ca (thick line) records for the time period of 1985–2004 from Timor: KP1.

fied univariate linear regression form  $y = mx + c$ , where  $y$  is the proxy measurement (e.g., Sr/Ca,  $\delta^{18}\text{O}$ ),  $x$  is the climate variable (e.g., SST),  $m$  is the regression coefficient, and  $c$  is the constant. These equations are used to convert

coral  $\delta^{18}\text{O}$  and Sr/Ca to temperature units. This method was first applied to coral proxies by McCulloch et al. (1994) and Gagan et al. (1998) (hereafter referred to as ANU method). The ANU method assumes that the inde-

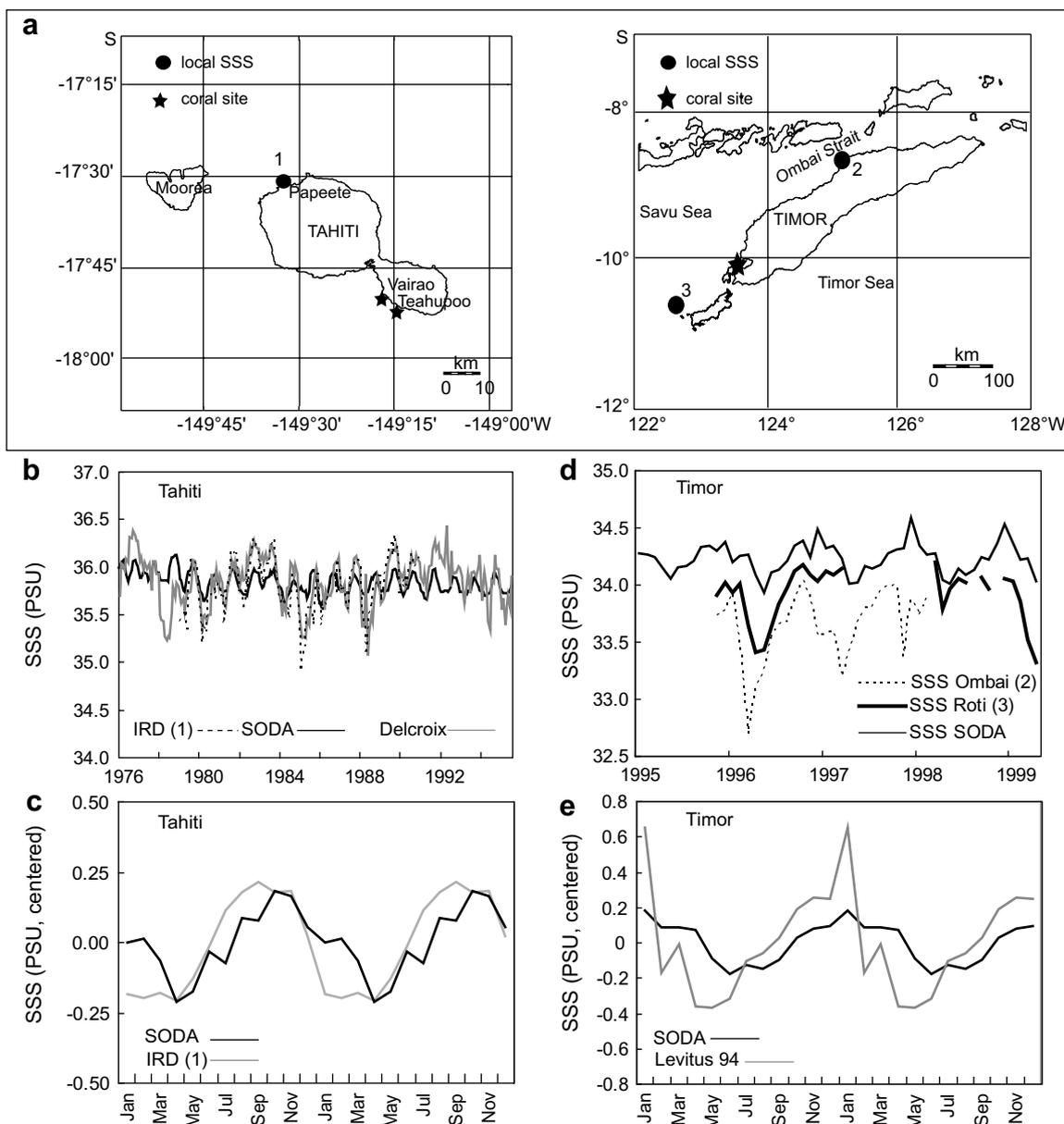


Fig. 4. (a) Location of map of Tahiti (left) and Timor (right). Available local salinity records are marked by black circles: (1) Papeete, Tahiti, (2) Ombai Strait, (3) Roti island. The coral drilling sites are indicated by a star. (b) Time series of monthly SSS SODA in the grid including Tahiti (149°2W 17°4S) (black line), SSS Delcroix (gray line), and SSS IRD (dashed line). (c) Monthly mean SSS at Tahiti: SSS SODA (black line) and SSS IRD (gray line). (d) Monthly time series of SSS measured at Timor and SSS SODA. (e) Monthly mean SSS at Timor: SSS SODA (black line) and SSS Levitus (gray line).

pendent variables ( $x$ ), i.e., SST, are free of error. We are aware, however, that the SST datasets, which are used as independent variables, are not free of error. This is a general problem of the linear regressions. Ren et al. (2002) saw the major problem in separating the SST and SSS signal in the estimate of the intercept. To omit the intercept values from the calculation of  $\delta^{18}\text{O}_{\text{sw}}$ , Ren et al. (2002) proposed to look at what they called the instantaneous changes of the proxies (e.g., the first time derivative). The general equation for  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions using the Ren et al. (2002) method is:

$$\begin{aligned} \Delta\delta^{18}\text{O}_{\text{coral}} &= \Delta\delta^{18}\text{O}_{\text{sst}} + \Delta\delta^{18}\text{O}_{\text{sw}} \\ &= (\partial\delta^{18}\text{O}_{\text{coral}}/\partial\text{SST})\Delta\text{SST} \\ &\quad + (\partial\delta^{18}\text{O}_{\text{coral}}/\partial\delta^{18}\text{O}_{\text{sw}})\Delta\delta^{18}\text{O}_{\text{sw}} \end{aligned} \quad (1)$$

where  $\Delta\delta^{18}\text{O}_{\text{sst}}$  ( $\Delta\delta^{18}\text{O}_{\text{sw}}$ ) is the SST ( $\delta^{18}\text{O}_{\text{sw}}$ ) contribution to coral  $\delta^{18}\text{O}$ .  $\partial\delta^{18}\text{O}_{\text{coral}}/\partial\text{SST}$  and  $\partial\delta^{18}\text{O}_{\text{coral}}/\partial\delta^{18}\text{O}_{\text{sw}}$  are the partial derivatives of coral  $\delta^{18}\text{O}$  with respect to SST and  $\delta^{18}\text{O}_{\text{sw}}$ , respectively. They represent the rate of change in coral  $\delta^{18}\text{O}$  with respect to the change of one variable, while the other variable is constant. The partial derivatives

of  $\delta^{18}\text{O}_{\text{coral}}$  and Sr/Ca with respect to SST are the slopes of the proxy-SST regression equations, i.e.,  $\gamma_1$  and  $\beta_1$ , respectively.  $\partial\text{Sr/Ca}/\partial\text{SST}$  or the partial derivative of Sr/Ca with respect to SST can be estimated based on the linear regression of Sr/Ca vs. SST. Similarly,  $\partial\delta^{18}\text{O}_{\text{coral}}/\partial\text{SST}$  can be estimated from the linear regression of coral  $\delta^{18}\text{O}$  vs. measured SST, provided that seawater  $\delta^{18}\text{O}$  does not change over this calibration interval.

Using the Ren et al. (2002) method, absolute  $\delta^{18}\text{O}_{\text{sw}}$  values are calculated by adding up all the instantaneous contributions to a reference value, i.e., the mean  $\delta^{18}\text{O}_{\text{sw}}$  value of a given location. However, the mean value of  $\delta^{18}\text{O}_{\text{sw}}$  is often poorly known as  $\delta^{18}\text{O}_{\text{sw}}$  measurements are scarce.

## 5.2. Centering method

In order to omit the intercept value (constant of regression), we can center the linear regression equation by removing the mean value from its variables (Draper and Smith, 1981). Centering is a standard method in regression analysis, but until now, it has not been used in the calculation of  $\delta^{18}\text{O}_{\text{sw}}$  from paired coral  $\delta^{18}\text{O}$  and Sr/Ca measurements. The Centering and the Ren et al. (2002) method have the same goal: to omit the intercept in the calculation of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$ . If measured coral  $\delta^{18}\text{O}$  is  $\delta^{18}\text{O}_{\text{coral}}$ , the SST contribution to  $\delta^{18}\text{O}_{\text{coral}}$  is  $\delta^{18}\text{O}_{\text{sst}}$  and the seawater  $\delta^{18}\text{O}$  contribution to  $\delta^{18}\text{O}_{\text{coral}}$  is  $\delta^{18}\text{O}_{\text{sw}}$ , we can define variations of  $\delta^{18}\text{O}_{\text{coral}}$  relative to the mean value of  $\delta^{18}\text{O}_{\text{coral}}$  (hereafter referred to as  $\Delta\delta^{18}\text{O}_{\text{C-center}}$ ) as the sum of  $\delta^{18}\text{O}_{\text{sst}}$  relative to the mean value of  $\delta^{18}\text{O}_{\text{sst}}$  (hereafter referred to as  $\Delta\delta^{18}\text{O}_{\text{sst-center}}$ ) and  $\delta^{18}\text{O}_{\text{sw}}$  relative to the mean value of  $\delta^{18}\text{O}_{\text{sw}}$  (hereafter referred to as  $\Delta\delta^{18}\text{O}_{\text{sw-center}}$ ). Thus,  $\Delta\delta^{18}\text{O}_{\text{sw-center}}$  can be calculated as:

$$\Delta\delta^{18}\text{O}_{\text{sw-center}} = \left( \delta^{18}\text{O}_{\text{coral}_i} - \overline{\delta^{18}\text{O}_{\text{coral}}} \right) - \gamma_1/\beta_1 (\text{Sr/Ca}_i - \overline{\text{Sr/Ca}}) \quad (2)$$

where  $\Delta\delta^{18}\text{O}_{\text{sw-center}}$  is the centered  $\delta^{18}\text{O}_{\text{sw}}$  contribution to  $\delta^{18}\text{O}_{\text{coral}}$ , Sr/Ca is measured coral Sr/Ca,  $\overline{\text{Sr/Ca}}$  is the mean value of measured Sr/Ca,  $\gamma_1$  is the regression slope of coral  $\delta^{18}\text{O}$  vs. SST, and  $\beta_1$  is the regression slope of coral Sr/Ca vs. SST.

## 6. COVARIANCE AND REGRESSION COEFFICIENTS IN A MULTIVARIATE DATASET

In most studies, the  $\delta^{18}\text{O}_{\text{coral}}$ -SST relationship is estimated via the ANU method, i.e., with a univariate linear regression of  $\delta^{18}\text{O}_{\text{coral}}$  vs. SST (e.g., McCulloch et al., 1994; Gagan et al., 1998; Gagan et al., 2000). However, coral  $\delta^{18}\text{O}$  is influenced concomitantly by SST and  $\delta^{18}\text{O}_{\text{sw}}$  (SSS). Therefore, if the ANU method is used for  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions from paired coral  $\delta^{18}\text{O}$  and Sr/Ca measurements, evidence should be given that at that particular location, the covariance between SST and SSS is negligible. [In statistics, covariance is the measure of how much two random variables vary together. If two variables tend to vary together (that is, when one of them is above its expected value, then the other variable tends to be above its expected value too), then the covariance between the two variables

will be positive. The more commonly used term correlation indicates the strength and direction of a linear relationship between two random variables. The popular Pearson product-moment correlation coefficient is obtained by dividing the covariance of the two variables by the product of their standard deviations].

If  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) variations are independent of SST, the effect of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) can be understood as an additional error. However, in the tropical oceans SST and  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) often co-vary (e.g., Gouriou and Delcroix, 2002), and thus the partial regression coefficient  $\gamma_1$  will be biased in the simple linear regression case of the ANU method, which estimates  $\gamma_1$  only from SST and coral  $\delta^{18}\text{O}$ . Thus,  $\gamma_1$  includes SST-covariant  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) variations and this biased parameter is used to calculate the 'residual'  $\delta^{18}\text{O}_{\text{sw}}$ . It is not the intercept, but the bias in the regression coefficient  $\gamma_1$  that causes problems in separating  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) and SST variability.

Here, we demonstrate the effect of correlation between SST and SSS on the estimates of the regression coefficients in a multivariate- and univariate dataset. We use simulated data and a stochastic model to illustrate this effect. We use the stochastic model  $y = Ax + Be$ , where  $y$  is the proxy signal (e.g.,  $\delta^{18}\text{O}_{\text{coral}}$  ( $y_1$ ) and Sr/Ca ( $y_2$ )),  $x$  is the climate signal (e.g., SSS ( $x_1$ ) and SST ( $x_2$ )), and  $e$  is the error. A and B is a transformation matrix  $2 \times 2$ , which determines the signal amplitude and controls the noise amplitude, respectively:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \quad B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

where  $a_{11}$  is the  $\delta^{18}\text{O}_{\text{coral}}$ -SSS relationship,  $a_{12}$  is the  $\delta^{18}\text{O}_{\text{coral}}$ -SST relationship,  $a_{21}$  is the Sr/Ca-SSS relationship, and  $a_{22}$  is the Sr/Ca-SST relationship. Example values chosen are:  $a_{11} = 0.5$ ,  $a_{12} = 1$ ,  $a_{21} = 0$ ,  $a_{22} = 1$ ;  $b_{22} = 1$ ,  $b_{11} = \text{sqrt}(a_{11} * a_{11} + a_{12} * a_{12} + 2 * a_{11} * a_{12} * \text{cor})$ . However, the noise components of  $b_{22}$  and  $b_{11}$  may vary between coral sites. Here,  $b_{22}$  is set to 1, which gives a signal to noise ratio of 1 (which is a conservative value of tropical coral proxies). The factor  $b_{11}$  depends on the correlation  $R$  between the two signals  $x_1$ ,  $x_2$ , such that the signal to noise ratio of  $y_1$  is also 1. Assuming that the noise of  $y_1$  and  $y_2$  is independent, we choose  $b_{12} = b_{21} = 0$ . Furthermore, we assume that  $y_1$  is influenced by two signals ( $x_1$ ,  $x_2$ ) and that  $y_2$  is influenced by one signal ( $x_2$ ). The proxy signal  $y_1$  and  $y_2$  can be written as:

$$y_1 = 0.5 * x_1 + 1 * x_2 + b_{11} * e_1 \\ y_2 = 0 * x_1 + 1 * x_2 + 1 * e_2$$

We generate random samples of signal  $x$  from a Gaussian noise process for correlations in  $x_1$  and  $x_2$  in the range of  $-0.9$   $-0.8$   $-0.7 \dots$  to  $0.9$ . The results show that the univariate and multivariate approach used in the reconstruction of  $\delta^{18}\text{O}_{\text{sw}}$  based on paired  $\delta^{18}\text{O}_{\text{coral}}$  and Sr/Ca measurement only yield the same regression coefficients when the correlation between SST and SSS is very small (Fig. 5). A correlation of 0.5 can lead to significant differences in the slope estimates. This would have immediate impact on the reconstructed SSS ( $\delta^{18}\text{O}_{\text{sw}}$ ) signals, which could lead to the misleading to the climatic interpretations.

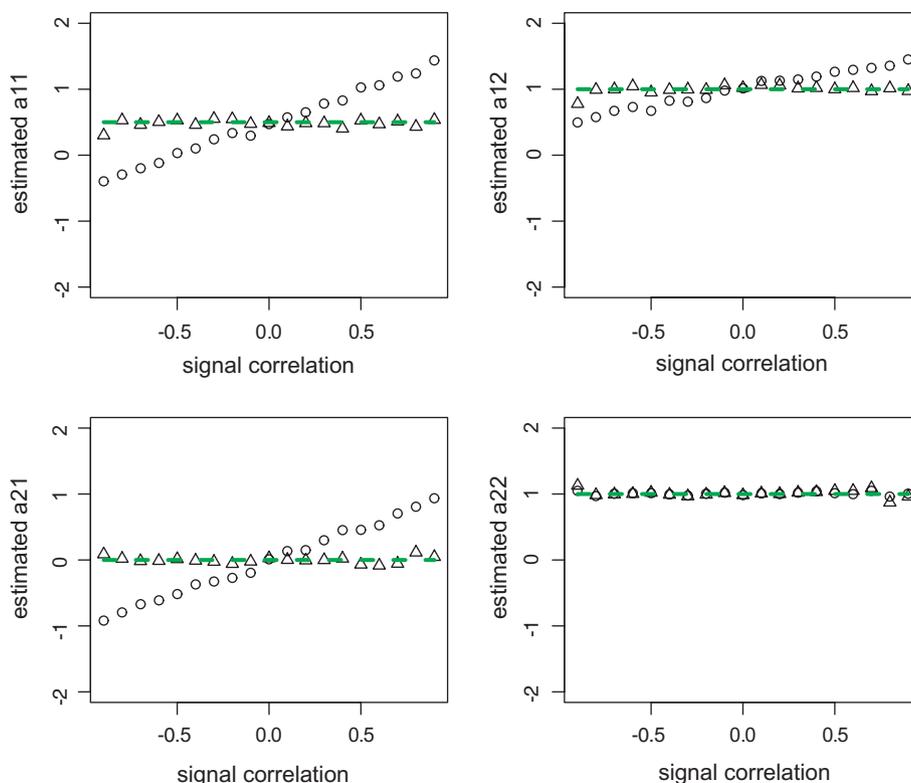


Fig. 5. The effect of correlation between SST and SSS on the slope values estimated by univariate and multivariate linear regression ( $a_{11}$ : coral  $\delta^{18}\text{O}$ –SSS,  $a_{12}$ : coral  $\delta^{18}\text{O}$ –SST,  $a_{21}$ : Sr/Ca–SSS,  $a_{22}$ : Sr/Ca–SST). Dashed line: true prescribed slope values. Triangles: slope values estimated by multivariate regression. Circles: slope values estimated by univariate linear regression. For zero correlation between SST and SSS, the slope values estimated with univariate and multivariate regression are identical. However, a correlation of 0.5 can lead to a significant bias in the  $\delta^{18}\text{O}$ –SST slope estimate if univariate linear regression equations are applied. This will in turn bias the  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) reconstruction. See text for discussion.

## 7. ERROR PROPAGATION

We calculate the error propagation of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  ( $\sigma$ ) including the analytical errors of the  $\delta^{18}\text{O}_{\text{coral}}$  and Sr/Ca measurements. This error estimate does not necessarily reflect the actual error of our  $\delta^{18}\text{O}_{\text{sw}}$  reconstruction. The actual error ( $e$ ) would be the sum of noise ( $\epsilon$ ) (e.g., the sum of all non-climatic factors that may influence the proxies) and the error propagation ( $\sigma$ ). Extensive environmental monitoring and many coral records are needed to accurately determine the noise component before we can calculate the actual error. However, the error propagation provides important constraints on  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions: we can definitely not resolve  $\delta^{18}\text{O}_{\text{sw}}$  variations that are smaller than the combined analytical uncertainties of coral  $\delta^{18}\text{O}$  and Sr/Ca measurements.

The individual errors of the measured physical parameters propagate through any calculation. If  $Y = f(\chi_1, \chi_2, \dots, \chi_i)$  and each  $X_i$  has its own associated standard error  $\sigma_{\chi_i}$ , the squared error propagation of  $Y$  is given by (see e.g., Bevington, 1969; Press et al., 1990):

$$\sigma^2 Y = \sum_{i=1}^n \left( \frac{\partial f}{\partial X_i} \right)^2 \sigma^2 X_i \quad (3)$$

when calculating  $\delta^{18}\text{O}_{\text{sw}}$  from measured coral  $\delta^{18}\text{O}$  and Sr/Ca, the covariance between the two variables can be

neglected, because the measurement accuracy of coral  $\delta^{18}\text{O}$  and Sr/Ca is un-related to each other. Based on Eq. (3), we can calculate the error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$ . The error of  $\delta^{18}\text{O}_{\text{sw}}$  estimated using the Ren et al. (2002) and centering method is calculated as follows:

$$\sigma_{\delta_{\text{sw}}}^2 = \sigma_{\delta_{\text{c}}}^2 + \left( \frac{\gamma_1}{\beta_1} \right)^2 \sigma_{\text{Sr/Ca}}^2 \quad (4)$$

where  $\sigma_{\delta_{\text{sw}}}$  is the error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$ ,  $\sigma_{\delta_{\text{c}}}$  is the error of measured  $\delta^{18}\text{O}_{\text{coral}}$ ,  $\sigma_{\text{Sr/Ca}}$  is the error of measured Sr/Ca,  $\gamma_1$  and  $\beta_1$  are the slopes of the linear regression of  $\delta^{18}\text{O}$  vs. SST and Sr/Ca vs. SST, respectively. Note that the error contributions from the means are negligible when averaged over a large sample size.

## 8. EXAMPLES: TAHITI AND TIMOR

### 8.1. Calibration Sr/Ca ( $\delta^{18}\text{O}$ ) vs. SST

We illustrate the univariate linear regression approach by calibrating coral Sr/Ca ( $\delta^{18}\text{O}$ ) with SST from the SODA dataset. Coral Sr/Ca ( $\delta^{18}\text{O}$ ) was regressed against SST using points defining seasonal maxima and minima in the records. This effectively eliminates possible slope biases due to seasonal-scale age model uncertainties of the proxy time series (Correge et al., 2004). For the sake of brevity,

we will only use the composite proxy records of TH1 and TH2 from Tahiti (hereafter referred to as  $\text{Sr}/\text{Ca}_{\text{TH12}}$  and  $\delta^{18}\text{O}_{\text{TH12}}$ ). The TH1 and TH2 proxy records are averaged after conversion to time. Averaging should reduce the noisiness of the proxy records as, for example, site-specific effects may bias single-core reconstructions. The regression equation (with 95% confidence levels) for monthly  $\text{Sr}/\text{Ca}_{\text{TH12}}$  vs. SST (1975–1995) is:

$$\text{Sr}/\text{Ca} = -0.063 \pm 0.004\text{SST} + 10.52 \pm 0.12$$

$$(R = 0.86, p < 0.001, \sigma = 0.04) \quad (5)$$

And for monthly  $\delta^{18}\text{O}_{\text{TH12}}$  vs. SST is:

$$\delta^{18}\text{O}_{\text{coral}} = -0.190 \pm 0.019\text{SST} + 0.67 \pm 0.51$$

$$(R = 0.85, p < 0.001, \sigma = 0.13) \quad (6)$$

At Tahiti, the slopes of the  $\text{Sr}/\text{Ca}$ - and the  $\delta^{18}\text{O}$ -SST relationships are consistent with published estimates.

At Timor, we obtain the following  $\text{Sr}/\text{Ca}_{\text{KP1}}(\delta^{18}\text{O}_{\text{KP1}})$ -SST regression equations:

$$\text{Sr}/\text{Ca} = -0.040 \pm 0.003\text{SST} + 9.83 \pm 0.09$$

$$(R = 0.89, p < 0.001, \sigma = 0.04) \quad (7)$$

$$\delta^{18}\text{O}_{\text{coral}} = -0.10 \pm 0.02\text{SST} - 2.02 \pm 0.59$$

$$(R = 0.68, p < 0.001, \sigma = 0.3) \quad (8)$$

At Timor, the slope of  $\text{Sr}/\text{Ca}$ -SST relationship is consistent with published estimates that range from  $-0.04$  to  $-0.08$  mmol/mol/ $^{\circ}\text{C}$  (Beck et al., 1992; de Villiers et al., 1994; Shen et al., 1996; de Villiers et al., 2002; Marshall and McCulloch, 2002; Alibert et al., 2003; Mitsuguchi et al., 2003). In contrast, the slope of  $\delta^{18}\text{O}$ -SST relationship is too low ( $-0.10 \pm 0.02\%$ / $^{\circ}\text{C}$ ) compared to published estimates ( $-0.15$  to  $-0.22\%$ / $^{\circ}\text{C}$ ; Weber and Woodhead, 1972; Wellington et al., 1996; Gagan et al., 1998; Juillet-Leclerc and Schmidt, 2001; Suzuki et al., 2005).

## 8.2. Reconstructing $\delta^{18}\text{O}_{\text{sw}}$ (SSS) at Tahiti and Timor

### 8.2.1. Methodologies of $\delta^{18}\text{O}_{\text{sw}}$ reconstructions, with examples from Tahiti

Here, we illustrate that  $\delta^{18}\text{O}_{\text{sw}}$  changes calculated using the Ren et al. (2002) and the centering method are identical. We use  $\text{Sr}/\text{Ca}_{\text{TH12}}$  and  $\delta^{18}\text{O}_{\text{TH12}}$  as an example. For  $\text{Sr}/\text{Ca}$ , we use the slope of the monthly  $\text{Sr}/\text{Ca}_{\text{TH12}}$  vs. SODA SST regression ( $\beta_1 = -0.063$  mmol/mol/ $^{\circ}\text{C}$ ). Published regression slopes of  $\delta^{18}\text{O}$  vs. SST in biological carbonates range from  $-0.15\%$ / $^{\circ}\text{C}$  to  $-0.23\%$ / $^{\circ}\text{C}$  (O'Neil et al., 1969; Bemis et al., 1998; von Langen et al., 2000; Spero et al., 2003). Corals show more or less the same range of  $\delta^{18}\text{O}$ -SST relationships ( $-0.15\%$ / $^{\circ}\text{C}$  to  $-0.22\%$ / $^{\circ}\text{C}$ ; Weber and Woodhead, 1972; Wellington et al., 1996; Gagan et al., 1998; Juillet-Leclerc and Schmidt, 2001; Suzuki et al., 2005). We use  $\gamma_1 = -0.18\%$ / $^{\circ}\text{C}$  (Gagan et al., 1998) for the coral  $\delta^{18}\text{O}$ -SST relationship. This value is a good average of published  $\delta^{18}\text{O}$ -SST slope values.

First, we calculate  $\delta^{18}\text{O}_{\text{sw}}$  using the method of Ren et al. (2002) (Fig. 6a). To reconstruct absolute values of  $\delta^{18}\text{O}_{\text{sw}}$ , Ren et al. (2002) add up their  $\delta^{18}\text{O}_{\text{sw}}$  contribution onto a reference value. The reference value should be the mean va-

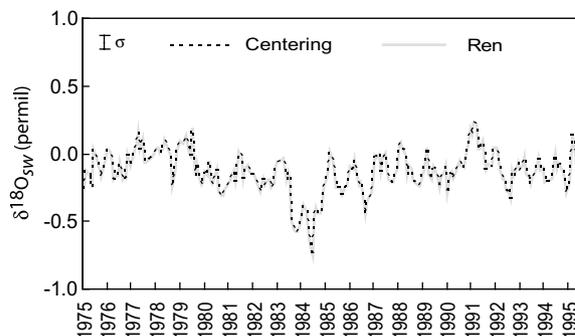


Fig. 6. Reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  derived from  $\text{Sr}/\text{Ca}_{\text{TH12}}$  and  $\delta^{18}\text{O}_{\text{TH12}}$ , calculated using the method of Ren et al. (2002), minus its mean value (thick gray line) and reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  derived from  $\text{Sr}/\text{Ca}_{\text{TH12}}$  and  $\delta^{18}\text{O}_{\text{TH12}}$  calculated with the centering method (thin black line).

lue of  $\delta^{18}\text{O}_{\text{sw}}$  at the site. Because we do not know the mean  $\delta^{18}\text{O}_{\text{sw}}$  at our coral sites, we arbitrarily set the reference value to 0. The reference value is needed to determine the absolute values of  $\delta^{18}\text{O}_{\text{sw}}$ . We then subtract the mean value of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  calculated with Ren et al. (2002) from reconstructed  $\delta^{18}\text{O}_{\text{sw}}$ . Thus, we obtain relative variations of  $\delta^{18}\text{O}_{\text{sw}}$  (Fig. 6, gray line).

We also calculate relative variations of  $\delta^{18}\text{O}_{\text{sw}}$  with the centering method. We use the same slope parameters for and as in the Ren et al. (2002) example. The results are shown in Fig. 6 (dashed line). We find that relative  $\delta^{18}\text{O}_{\text{sw}}$  variations calculated with Ren et al. (2002) and centering are identical (Fig. 6). However, the centering method involves much simpler calculations than Ren et al. (2002), and is a standard method in linear regression analysis (Draper and Smith, 1981). Therefore, it should be the method of choice for  $\delta^{18}\text{O}_{\text{sw}}$  reconstructions from paired coral  $\text{Sr}/\text{Ca}$  and  $\delta^{18}\text{O}$  measurements.

### 8.2.2. Monthly $\delta^{18}\text{O}_{\text{sw}}$ (SSS) at Tahiti and analytical errors

We calculate the error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  from paired  $\text{Sr}/\text{Ca}_{\text{TH12}}$  and  $\delta^{18}\text{O}_{\text{TH12}}$  measurements. The standard deviation of measured coral  $\delta^{18}\text{O}$  and  $\text{Sr}/\text{Ca}$  is  $\sigma_{\delta\text{c}} = \pm 0.06$  ‰ ( $1\sigma$ ) and  $\sigma_{\text{Sr}/\text{Ca}} = \pm 0.01$  mmol/mol ( $1\sigma$ ), respectively. The slope of the  $\delta^{18}\text{O}$ -SST relationship is  $\gamma_1 = -0.18$  ‰/ $^{\circ}\text{C}$  (Gagan et al., 1998). The slope of the  $\text{Sr}/\text{Ca}$ -SST relationship is  $\beta_1 = -0.063$  mmol/mol/ $^{\circ}\text{C}$  ( $\text{Sr}/\text{Ca}_{\text{TH12}}$  vs. SODA). For the centering and Ren et al. (2002) method, the error of  $\delta^{18}\text{O}_{\text{sw-TH12}}$  is calculated as follows:  $\sigma_{\Delta\delta\text{sw}}^2 = \sigma_{\delta\text{c}}^2 + \sigma_{\text{Sr}/\text{Ca}}^2 (\gamma_1/\beta_1)^2 = 0.06^2 + 0.01^2 (\text{mmol/mol})^2 (-0.18/ -0.063 \text{ mmol/mol})^2 = \pm 0.0044\%$ , thus,  $\sigma_{\Delta\delta\text{sw}} = \pm 0.066\%$ .

Since we omit the intercept values of the linear regression equations from the  $\delta^{18}\text{O}_{\text{sw}}$  calculation using either Ren et al. (2002) or centering, we also omit the intercept error. By choosing temperature as independent variable, the slope and the regression errors are small, and can be neglected. This results in a relatively small error of the  $\delta^{18}\text{O}_{\text{sw}}$  reconstruction. Note, however, that this error only applies to relative  $\delta^{18}\text{O}_{\text{sw}}$  variations. Furthermore, we would expect the actual error to be larger, as the corals are also influenced by non-climatic noise, such as biological

factors that influence the incorporation of the proxies during coral growth (e.g., Meibom et al., 2006; Sinclair et al., 2006).

Fig. 7 compares the monthly ( $\delta^{18}\text{O}_{\text{sw-TH12}}$ ) reconstruction with SSS from the SODA dataset. The correlation between the monthly time series of  $\delta^{18}\text{O}_{\text{sw-TH12}}$  and SSS SODA is low ( $R = 0.33$ ) (Fig. 7a). In almost all years, seasonal maxima and minima of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  and SSS do not match (Fig. 7a). Fig. 7b shows the mean seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  to be expected at Tahiti. The  $\delta^{18}\text{O}_{\text{sw}}$  cycle was

calculated from SSS SODA, which was converted to  $\delta^{18}\text{O}_{\text{sw}}$ -units by assuming an  $\delta^{18}\text{O}_{\text{sw}}$ -SSS slope of  $0.24\text{‰}/\text{psu}$ . SSS SODA shows seasonal cycle of  $0.32\text{ psu}$ , which would correspond to  $0.08\text{‰}$   $\delta^{18}\text{O}_{\text{sw}}$  (Fig. 7b). Other instrumental SSS datasets show similar seasonal variations (see Fig. 4c). We have also plotted the analytical error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  ( $\sigma_{\Delta\delta\text{sw}} = \pm 0.066\text{‰}$ ) in Fig. 7b. For seasonal-scale maxima and minima, the error bars overlap, i.e., the analytical error of our  $\delta^{18}\text{O}_{\text{sw}}$  reconstruction is on the same order of magnitude as the mean seasonal cycle

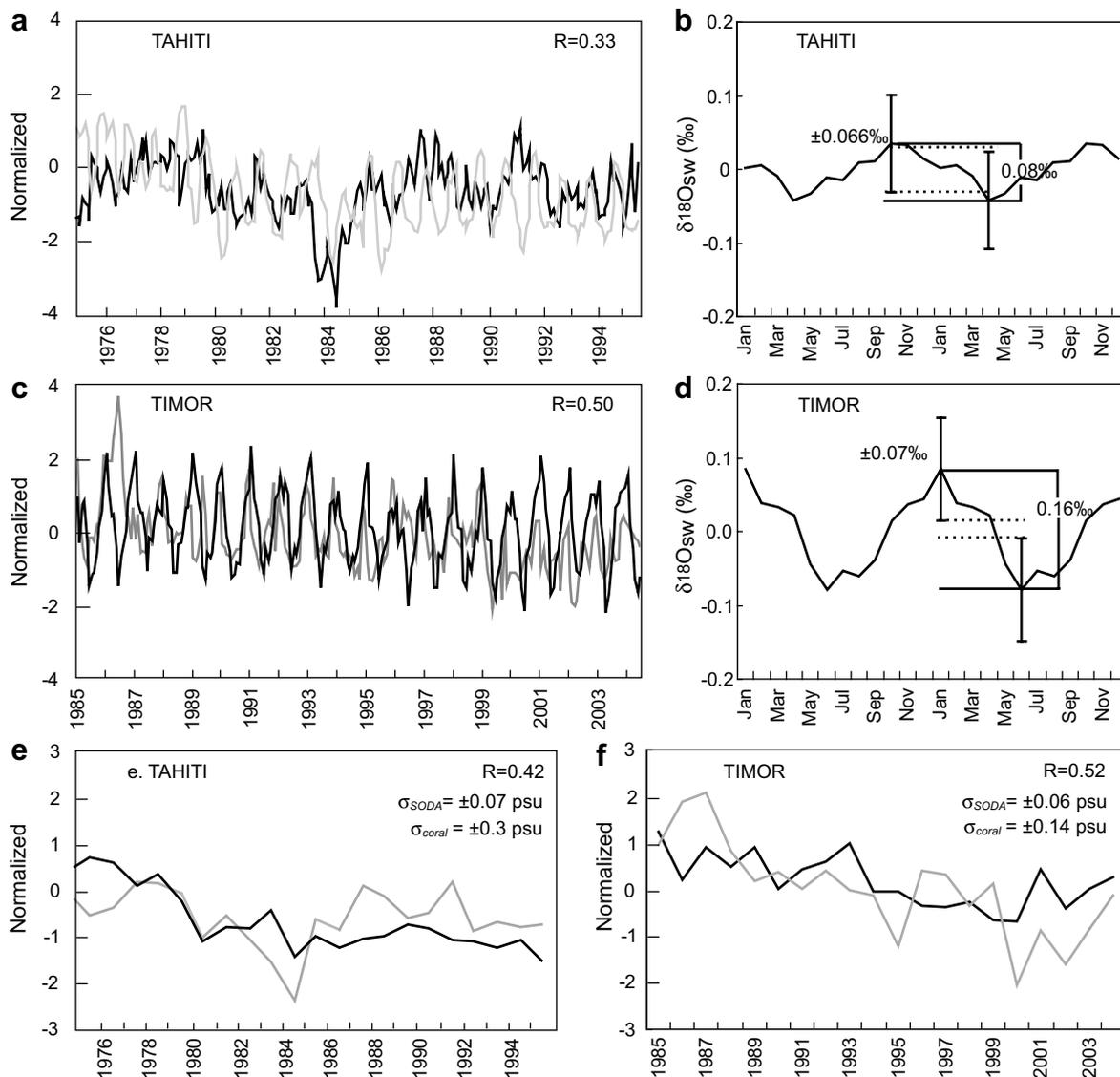


Fig. 7. (a) Monthly reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  (gray line) and SSS SODA (black line) at Tahiti.  $\delta^{18}\text{O}_{\text{sw}}$  is calculated using centering. Regression coefficients used:  $\gamma_1 = -0.18\text{‰}/\text{°C}$ ,  $\beta_1 = -0.063\text{ mmol/mol}/\text{°C}$ . (b) Mean monthly  $\delta^{18}\text{O}_{\text{sw}}$  contribution to measured coral  $\delta^{18}\text{O}$  at Tahiti.  $\delta^{18}\text{O}_{\text{sw}}$  is estimated from SSS SODA, assuming a  $\delta^{18}\text{O}_{\text{sw}}$ -SSS relationship of  $0.24\text{‰}/\text{psu}$ . The error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  is indicated (error bar  $\sigma = \pm 0.066\text{‰}$ ). Note that the error bars for seasonal maxima and minima overlap, as the error is larger than the mean seasonal amplitude of  $\delta^{18}\text{O}_{\text{sw}}$  variations ( $0.08\text{‰}$ ). (c) Monthly reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  (gray line) and SSS SODA (black line) at Timor.  $\delta^{18}\text{O}_{\text{sw}}$  is calculated using centering. Regression coefficients used:  $\gamma_1 = -0.18\text{‰}/\text{°C}$ ,  $\beta_1 = -0.04\text{ mmol/mol}/\text{°C}$ . (d) Mean monthly  $\delta^{18}\text{O}_{\text{sw}}$  contribution to measured coral  $\delta^{18}\text{O}$  at Timor.  $\delta^{18}\text{O}_{\text{sw}}$  is estimated from SSS SODA, assuming a  $\delta^{18}\text{O}_{\text{sw}}$ -SSS relationship of  $0.44\text{‰}/\text{psu}$ . The error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  is indicated (error bar  $\sigma = \pm 0.07\text{‰}$ ). Note that the error bars for seasonal maxima and minima do not overlap, as the error is smaller than the mean seasonal amplitude of  $\delta^{18}\text{O}_{\text{sw}}$  variations ( $0.16\text{‰}$ ). (e and f) Annual mean reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  (gray line) and SSS SODA (black line) for (e) Tahiti and (f) Timor. See text for discussion.

of  $\delta^{18}\text{O}_{\text{sw}}$  to be expected at Tahiti. Thus, we cannot resolve the seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  at Tahiti, and the correlation between monthly  $\delta^{18}\text{O}_{\text{sw}}$  and SSS is low.

Please note, however, that the slope obtained with our seasonal  $\delta^{18}\text{O}_{\text{TH12}}$ –SST calibration ( $-0.19 \text{ ‰}/^\circ\text{C}$ ) matches published estimates of coral  $\delta^{18}\text{O}$  vs. SST. This already indicates that seasonal  $\delta^{18}\text{O}_{\text{sw}}$  variations at Tahiti are too small to measurably affect coral  $\delta^{18}\text{O}$ . Theoretically it would be possible to apply a univariate regression of  $\delta^{18}\text{O}$  vs. SST to reconstruct  $\delta^{18}\text{O}_{\text{sw}}$ , as  $\delta^{18}\text{O}_{\text{sw}}$  variations appear to be negligible over the calibration period (see Huppert and Solow, 2004), but at least on a seasonal time scale, it would not be possible to actually reconstruct  $\delta^{18}\text{O}_{\text{sw}}$ .

### 8.2.3. Monthly $\delta^{18}\text{O}_{\text{sw}}$ (SSS) at Timor and analytical errors

Here, we will show that at Timor, the seasonal cycle of surface salinity can be resolved by paired  $\delta^{18}\text{O}$  and Sr/Ca measurements. We apply the centering method to reconstruct  $\delta^{18}\text{O}_{\text{sw}}$  from coral  $\delta^{18}\text{O}_{\text{KP1}}$  and Sr/Ca<sub>KP1</sub>. We insert the published slope value of the  $\delta^{18}\text{O}$ –SST relationship for  $\gamma_1$  ( $-0.18 \text{ ‰}/^\circ\text{C}$ ), because the calibration slope of  $\delta^{18}\text{O}_{\text{KP1}}$  vs. SST is too low compared to published estimates ( $-0.1 \pm 0.03 \text{ ‰}/^\circ\text{C}$ ) (this is to be expected, as on a seasonal scale, maximum SST and maximum SSS coincide). For Sr/Ca, we use the calibration slope of coral Sr/Ca<sub>KP1</sub>–SST ( $\beta_1 = -0.04 \text{ mmol/mol}/^\circ\text{C}$ ). The analytical uncertainty is  $\sigma_{\delta c} = \pm 0.06 \text{ ‰}$  ( $\sigma_1$ ) for  $\delta^{18}\text{O}$  coral, and  $\sigma_{\text{Sr/Ca}} = \pm 0.01 \text{ mmol/mol}$  ( $\sigma_2$ ) for Sr/Ca. Thus, the error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  at Timor is:  $\sigma_{\Delta\delta\text{sw}}^2 = \sigma_{\delta c}^2 + \sigma_{\text{Sr/Ca}}^2 (\gamma_1/\beta_1)^2 = 0.06^2 \text{ ‰}^2 + 0.01^2 (\text{mmol/mol})^2 (-0.18 \text{ ‰}/^\circ\text{C} / -0.04 \text{ mmol/mol}/^\circ\text{C})^2 = \pm 0.0056 \text{ ‰}^2$   $\sigma_{\Delta\delta\text{sw}} = \pm 0.07 \text{ ‰}$ .

Reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  from Sr/Ca<sub>KP1</sub> and  $\delta^{18}\text{O}_{\text{KP1}}$  co-varies in phase with SSS SODA (Fig. 7c). The correlation between monthly reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  and SSS SODA is high ( $R = 0.5$ ). Fig. 7d shows the expected mean seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  at Timor. The  $\delta^{18}\text{O}_{\text{sw}}$  cycle was calculated from SSS SODA, and converted to  $\delta^{18}\text{O}_{\text{sw}}$ -units using a  $\delta^{18}\text{O}_{\text{sw}}$ –SSS slope of  $0.44 \text{ ‰}/\text{psu}$  (Schmidt, 1999; data available at <http://data.giss.nasa.gov/cgi-bin/o18data>;  $110^\circ\text{E}$ – $130^\circ\text{E}$ ,  $20^\circ\text{N}$ – $30^\circ\text{S}$ ). SSS SODA shows a seasonal cycle of  $0.37 \text{ psu}$ , which would correspond to  $0.16 \text{ ‰}$   $\delta^{18}\text{O}_{\text{sw}}$  (Fig. 7d). Instrumental SSS measured at Roti and Ombai indicates even larger seasonal variations ( $>0.5 \text{ psu}$ , see Fig. 4e), but the time series are short. In Fig. 7d, we have also plotted the analytical error of reconstructed  $\delta^{18}\text{O}_{\text{sw}}$  at Timor ( $\sigma_{\Delta\delta\text{sw}} = \pm 0.07 \text{ ‰}$ ). The error bars of the seasonal maxima and minima do not overlap, i.e., the analytical error of our  $\delta^{18}\text{O}_{\text{sw}}$  reconstruction is smaller than the mean seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  at Timor. Thus, we can resolve the seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$ . Note, however, that the slope of the univariate  $\delta^{18}\text{O}$ –SST regression (Eq. (8)) is biased due to seasonal-scale, SST-covariant changes of  $\delta^{18}\text{O}_{\text{sw}}$ . The slope value obtained is too low, because maximum SST coincides with maximum SSS, and with the slope parameters being negative ( $\delta^{18}\text{O}$ –SST) and positive ( $\delta^{18}\text{O}_{\text{sw}}$ –SSS), SSS dampens the SST signal in the coral  $\delta^{18}\text{O}$ . According to Huppert and Solow (2004), it would not be possible to reconstruct  $\delta^{18}\text{O}_{\text{sw}}$  at Timor.

## 9. ANNUAL MEAN RECONSTRUCTED $\Delta^{18}\text{O}_{\text{sw}}$ (SSS)

An important aspect of coral-based climate studies is the reconstruction of interannual to decadal/multidecadal variations. In this context, it is important to assess the reliability of annual mean  $\delta^{18}\text{O}_{\text{sw}}$  estimates, and this is difficult due to the shortness of instrumental SSS data. Here, we compare annual mean  $\delta^{18}\text{O}_{\text{sw}}$  estimates of Tahiti and Timor with SSS SODA (Fig. 7e and f). We chose SSS SODA, because only SODA provides a continuous time series of SSS at both sites. We are aware, however, that the SODA dataset may have some problems, particularly at interannual time scales (see Fig. 4 and Section 4), and therefore our results should be viewed with some caution.

Annual mean  $\delta^{18}\text{O}_{\text{sw}}$  values are computed from a number of independent  $\delta^{18}\text{O}_{\text{sw}}$  estimates, and thus the analytical uncertainty of annual mean  $\delta^{18}\text{O}_{\text{sw}}$  reduces according to the formula:  $\sigma_{\text{Total}} = (\sigma^2/N)^{1/2}$ , where  $\sigma$  is the analytical error of the single proxy measurements, and  $N$  is the number of independent measurements (e.g., Bevington, 1969). For example, the analytical uncertainty for annual mean  $\delta^{18}\text{O}_{\text{sw-TH12}}$  reduces to  $\pm 0.019 \text{ ‰}$  or  $\pm 0.08 \text{ psu}$  (if we assume that annual mean  $\delta^{18}\text{O}_{\text{sw-TH12}}$  is calculated from 12 independent measurements; for 24 independent measurements the analytical uncertainty would be even lower). The analytical uncertainty for annual mean  $\delta^{18}\text{O}_{\text{sw-KP1}}$  reduces to  $\pm 0.02 \text{ ‰}$  (assuming  $\delta^{18}\text{O}_{\text{sw-KP1}}$  annual mean is calculated for 12 independent measurements).

According to Gouriou and Delcroix (2002) interannual variations of SSS in the Southwestern tropical Pacific, where Tahiti is located, are proportionally larger with respect to SST than on a seasonal scale. The standard deviation of annual mean SSS is  $\sigma = \pm 0.19 \text{ psu}$  in the historical record of Gouriou and Delcroix (2002), and  $\pm 0.07 \text{ psu}$  in SODA during the period of 1976–1995. Given the small analytical uncertainty of annual mean  $\delta^{18}\text{O}_{\text{sw}}$  estimates, annual mean SSS variations should measurably affect the skeletal chemistry of the Tahiti corals. Fig. 7e compares annual mean  $\delta^{18}\text{O}_{\text{sw-TH12}}$  with SSS from SODA. The correlation is  $R = 0.42$  and  $\delta^{18}\text{O}_{\text{sw-TH12}}$  co-varies with SSS SODA. Both series show a decrease of salinity/ $\delta^{18}\text{O}_{\text{sw}}$  in 1984/85 which indicates a freshening of surface waters.

The Indonesian region, on an annual scale, experiences warm and wet conditions. Lowest salinity is found in the western part of Indonesia extending from the Java sea to the South China sea. This fresh water flows through the ITF exit passages, but water transport changes seasonally. At Ombai strait (Timor), one of the main exit passages of the ITF, the annual cycle dominates the SST and SSS signal (Sprintall et al., 2003). Fig. 7f compares annual mean values of  $\delta^{18}\text{O}_{\text{sw-KP1}}$  and SSS SODA. The correlation between the two time series is high ( $R = 0.52$ ), and both series show a similar trend suggesting a freshening of surface waters since 1984 (Fig. 7f).

However, at both Tahiti and Timor the variance of annual mean SSS SODA is lower than the variance of reconstructed SSS from the corals (see Fig. 7e and f), although using the known (and presumably correct) slope for the coral  $\delta^{18}\text{O}$ –SST, as well as for the  $\delta^{18}\text{O}_{\text{sw}}$ –SSS relationship should yield the correct variations of local  $\delta^{18}\text{O}_{\text{sw}}$  and

SSS. The instrumental data of SSS available for the coral sites (Gouriou and Delcroix, 2002; Sprintall et al., 2003) suggest that SODA may underestimate the variance. Clearly, if we want to reduce the uncertainties of quantitative  $\delta^{18}\text{O}_{\text{sw}}$  and SSS reconstructions from corals, we need much better instrumental data that can only be obtained during long-term monitoring programs.

## 10. CONCLUSIONS

The ANU method for deriving  $\delta^{18}\text{O}_{\text{sw}}$  from paired coral  $\delta^{18}\text{O}$  and Sr/Ca measurements should not be used in areas where SST-covariant variations in  $\delta^{18}\text{O}_{\text{sw}}$  and SSS occur, because this would lead to a bias in the slope of the  $\delta^{18}\text{O}$ –SST relationship, since coral  $\delta^{18}\text{O}$  is calibrated with SST only. This biased slope would in turn lead to a systematic bias of  $\delta^{18}\text{O}_{\text{sw}}$  and SSS reconstructions. At Timor, we were able to identify such a bias in the coral  $\delta^{18}\text{O}$ –SST relationship. We further used simulated proxy data and a stochastic model to demonstrate the covariance problem in the univariate regression of coral  $\delta^{18}\text{O}$ –SST. The slope values obtained by univariate linear regression will be unbiased only when the covariance between two climate signals affecting one proxy is small.

The method of Ren et al. (2002) and the centering method proposed in this study omit the intercept values of the  $\delta^{18}\text{O}$ –SST and Sr/Ca–SST regression equations used for the calculation of  $\delta^{18}\text{O}_{\text{sw}}$ . Thus, it is possible to insert the known slope of the  $\delta^{18}\text{O}$  (Sr/Ca)–SST relationship and to calculate relative variations of  $\delta^{18}\text{O}_{\text{sw}}$  even at sites where SST-covariant variations in  $\delta^{18}\text{O}_{\text{sw}}$  and SSS occur. Practically, the Ren et al. (2002) and the centering method provide the same results. However, the Ren et al. (2002) method requires much more complicated mathematical calculations than centering, which is a standard method used to omit the intercept in linear regression analysis.

Note at Tahiti, we obtain the correct slope estimate for the  $\delta^{18}\text{O}$ –SST relationship in a univariate linear regression, but seasonal-scale changes in  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) are too small to be resolved with paired  $\delta^{18}\text{O}$  and Sr/Ca measurements. The error ( $\sigma$ ) of  $\delta^{18}\text{O}_{\text{sw}}$  calculated from coral  $\delta^{18}\text{O}_{\text{coral-TH12}}$  and Sr/Ca<sub>TH12</sub> is larger than the seasonal mean cycle of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS). At Timor, the slope of the  $\delta^{18}\text{O}$ –SST relationship obtained in a univariate linear regression is biased due to the large seasonal-scale variations of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS). Nevertheless, seasonal-scale variations of  $\delta^{18}\text{O}_{\text{sw}}$  (SSS) can be resolved when the known  $\delta^{18}\text{O}$ –SST relationship is used. At Timor, the error propagation ( $\sigma$ ) of  $\delta^{18}\text{O}_{\text{sw}}$  calculated from the paired  $\delta^{18}\text{O}$  and Sr/Ca records is lower ( $\sigma\Delta\delta_{\text{sw}} = \pm 0.07\text{‰}$ ) than the amplitude of the mean seasonal cycle of  $\delta^{18}\text{O}_{\text{sw}}$  (0.16‰).

On an annual mean scale, the error of  $\delta^{18}\text{O}_{\text{sw}}$  reduces because we average a large number of independent estimates. At Tahiti, annual mean  $\delta^{18}\text{O}_{\text{sw-TH12}}$  follows SSS from SODA, and both records indicate a freshening of surface waters in 1984/1985. At Timor, annual mean  $\delta^{18}\text{O}_{\text{sw-KP1}}$  shows a gradual freshening over the past 20 years. We note, however, that on an annual mean scale, the variance of SSS inferred from the Tahiti and Timor corals is larger than indicated by SSS SODA. This may reflect problems in the

SODA reanalysis. In order to obtain reliable, quantitative salinity reconstructions from corals we will need much better instrumental data of  $\delta^{18}\text{O}_{\text{sw}}$  and SSS that can only be obtained through long-term monitoring programs.

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