Supplementary Information to Southern Ocean sea surface temperature synthesis: Part 2. Penultimate glacial - last interglacial

David Chandler and Petra Langebroek
NORCE Norwegian Research Centre, Bjerknes Centre for Climate Research, Bergen, Norway

S1 Recent SST syntheses relevant to the Southern Ocean

Table S1.1: Comparison of recent SST syntheses relevant to the Southern Ocean. Abbreviations: AIS Antarctic Ice Sheet; GrIS Greenland Ice Sheet; A alkenones, C Dinoflagellate cysts; D diatom assemblage; G glycerol dialkyl glycerol tetraethers; F foraminifera assemblage; M foraminiferal Mg/Ca ratio; R radiolarian assemblage. Chronologies are LR04 (Lisiecki and Raymo, 2005); Speleo-Age (Barker et al., 2005); AICC2012 (Antarctic Ice Core Chronology: Bazin et al., 2013; Veres et al., 2013); and LS16 (Lisiecki and Stern, 2016). Notes: (a) The errors are not those reported by the authors, instead they are the mean and 95% confidence intervals calculated from contributing sites south of 40°S. These data were extracted from their supplementary online materials. (b) Non-drift-corrected anomalies.

	Capron et al. (2014)	**Hoffman et al. (2017)**	**Turney et al. (2020)**	**This study**
Region	S. Ocean 40 to 57°S; N. Atlantic; AIS & GrIS.	Global oceans 68°N to 51°S	Global oceans 72°N to 55°S	S. Ocean 40 to 57°S
Time period, resolution	130 to 115 ka, 5 kyr resolution.	130 to 115 ka, 0.1 kyr resolution.	'LIG' mean, 'Early LIG', 140 to 135 ka mean.	200 to 0 ka, 2 kyr resolution.
Records south of 40°S	2 annual 15 summer	12 annual 7 summer	28 annual 25 summer	29 annual 27 summer
SST proxies	A, D, F, M, R	A, D, F, M, R	A, D, F, G, M R	A, D, F, M (C, G, R excluded)
Calibrations	All as in original publication.	As in original publication, except Müller et al. (1998) for alkenones, Anand et al. (2003) for Mg/Ca.	All as in original publication.	A, F, M revised (see Part 1). D as in original publication.
Age models	SST aligned with EDC δD.	Selected reference core SSTs aligned with EDC δD. Other cores aligned with reference cores by benthic δ^{18}O.	Various: δ^{18}O, sediment $CaCO_3$ content, and others; target not specified.	Benthic δ^{18}O aligned with LS16 regional stack. Planktic δ^{18}O used if benthic δ^{18}O not available.
Chronology	AICC2012	Speleo-Age	Not reported	LS16
Modern SST reference	WOA1998, 10 m (Conkright et al., 1998)	HadISST1.1 (Rayner et al., 2003)	HadISST1.1 (Rayner et al., 2003)	WOA2018, surface (Locarnini et al., 2018)
Mean annual SST anomaly at sites south of 40°S [°C]				
PGM	—	—	$-3.1 \pm 2.1^{(a,b)}$	-3.6 ± 1.1
130 ka	—	$+1.8 \pm 3.2^{(a)}$	)	$+1.1 \pm 1.1$
125 ka	—	$+2.0 \pm 3.1^{(a)}$	) $+0.7 \pm 1.3^{(a,b)}$	$+1.6 \pm 1.1$
120 ka	—	$+1.4 \pm 3.0^{(a)}$	)	$+0.2 \pm 0.7$
115 ka	—	$-0.0 \pm 2.9^{(a)}$	)	-0.9 ± 0.8
Mean summer SST anomaly at sites south of 40°S [°C]				
PGM	—	—	—	-4.0 ± 1.2
130 ka	$+1.5 \pm 0.9^{(a)}$	$+0.9 \pm 2.4^{(a)}$	)	$+0.9 \pm 1.1$
125 ka	$+1.3 \pm 1.0^{(a)}$	$+0.6 \pm 3.0^{(a)}$	) $-0.3 \pm 0.8^{(a,b)}$	$+1.9 \pm 1.3$
120 ka	$+1.0 \pm 0.9^{(a)}$	$-0.6 \pm 2.8^{(a)}$	)	$+0.7 \pm 0.9$
115 ka	$-0.5 \pm 0.9^{(a)}$	$-2.1 \pm 2.5^{(a)}$	)	-0.7 ± 0.9

S2 Dating

Here we justify our preference for only using age models based on foraminiferal δ^{18}O, rather than using SST itself (Capron et al., 2014) or a combination of both (Hoffman et al., 2017). We consider regional variability in benthic foraminiferal δ^{18}O, the relative contributions of seawater temperature and seawater δ^{18}Ow signals in foraminiferal calcite δ^{18}O, and the validity of using planktic foraminiferal δ^{18}O in addition to benthic foraminiferal δ^{18}O.

S2.1 Regional synchronicity in benthic foraminiferal δ^{18}O

In our study region, published age models based on δ^{18}O were often aligned with a global benthic δ^{18}O stack, for example SPECMAP (Imbrie et al., 1984) or LR04 (Lisiecki and Raymo, 2005), under the assumption of globally synchronous changes in benthic δ^{18}O on millennial time scales. More recent analysis with a much larger number of sites has enabled a more detailed evaluation of regional differences in the timing of δ^{18}O changes over the last 150 ka (Lisiecki and Stern, 2016). Selecting relevant regions from their study (here abbreviated as LS16) does indeed show some notable offsets: firstly between their revised global stack and the older LR04 (Fig. S2.1, top panel), and secondly between different ocean basins (Fig. S2.1, bottom panel). In the former case, LR04 lags the global LS16 by ∼2 kyr during the early LIG. In the latter case, individual basins show quite different δ^{18}O responses over the LIG, leading to inter-basin differences of up to 2.5 kyr between the timings of the three highlighted events. Therefore, to take advantage of this newer chronology, we should transfer published age models for the selected sediment cores onto the LS16 regional stacks, rather than using the global LR04 chronology. In practice we find this makes little difference to the final result (see Table 1 in the main text).

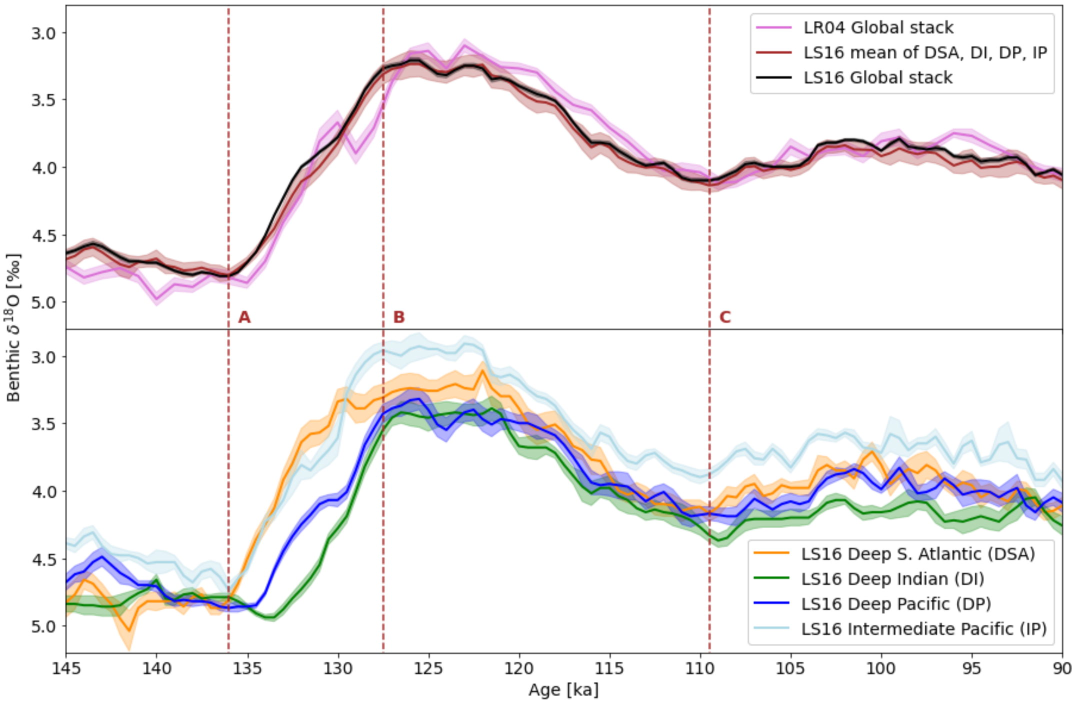

Figure S2.1: Regional and global averages of benthic δ^{18}O reported by Lisiecki and Raymo (2005) and Lisiecki and Stern (2016) (abbreviated LR04 and LS16, respectively). The top panel shows the LR04 global stack, LS16 global stack, and LS16 average over basins relevant to our study region (deep S. Atlantic, deep Indian, deep Pacific, intermediate Pacific). This 'regional stack' is simply the unweighted arithmetic mean of the contributing individual regions, and is seen to be indistinguishable from the global stack (black line). The bottom panel shows the individual basins contributing to the regional mean. Shading is 1 standard error. Vertical lines A, B, C correspond to key events in the LS16 global stack, as listed in Table S1.1

Table S2.1: Timing of events A, B and C in the benthic stacks shown in Fig. S2.1. These correspond to the vertical dashed lines in that figure. Regions are deep South Atlantic (DSA), deep Indian (DI), deep Pacific (DP) and intermediate Pacific (IP).

	Resolution (kyr)	**Event A**	**Event B**	**Event C**
LR04 (global)	1	136	125	108
LS16 (global)	0.5	136.0	127.5	109.5
LS16 (DSA)	0.5	134.5	127.0	109.5
LS16 (DI)	0.5	133.5	126.5	109.0
LS16 (DP)	0.5	134.5	127.5	108.5
LS16 (DI)	0.5	136.0	128.0	110.0

S2.2 Superimposed seawater $\delta^{18}\mathrm{O_w}$ and temperature signals in foraminiferal $\delta^{18}\mathrm{O_c}$

Foraminiferal calcite δ^{18}O (which we will call $\delta^{18}\mathrm{O_c}$ here) depends partly on water temperature and on water $\delta^{18}\mathrm{O_w}$ (Urey et al., 1951; Shackleton, 1974), according to the widely-used paleotemperature equation:

$$T = 16.9 - 4.2(\delta^{18}\mathrm{O_c} - \delta^{18}\mathrm{O_w}) + 0.13(\delta^{18}\mathrm{O_c} - \delta^{18}\mathrm{O_w})^2. \tag{S2.1}$$

Here, subscripts c and w refer to calcite and seawater, respectively. Sometimes $\delta^{18}\mathrm{O_c}$ is corrected for species-specific vital effects by adding an offset (e.g., Rodríguez-Sanz et al., 2012).

We can use Eq. S2.1 to estimate the magnitude of the local water temperature signal in glacial-interglacial changes in Southern Ocean benthic and planktic $\delta^{18}\mathrm{O_c}$, and then assess whether this might contribute significant offsets in our age models. First, by setting $D = \delta^{18}\mathrm{O_c} - \delta^{18}\mathrm{O_w}$, then from Eq. S2.1:

$$16.9 - T - 4.2D + 0.13D^2 = 0 \tag{S2.2}$$

Solving Eq. S2.2 for D gives

$$D = [4.2 \pm \sqrt{4.2^2 - 4 \times (16.9 - T) \times 0.13}]/0.26 \tag{S2.3}$$

This is an exact solution, but more conveniently there is a good linear approximation for the relevant temperature range $-2 < T < 15$°C:

$$D \approx -0.289T + 4.67 \tag{S2.4}$$

In the Southern Ocean, a linear relationship may indeed be more appropriate for *G. bulloides* and *N. pachyderma* (Mulitza et al., 2003), which are the two planktic species used in age models for that region. With our linear relationship (Eq. S2.4) and above definition of D, we now have a linear relationship linking foraminiferal $\delta^{18}\mathrm{O_c}$ with water temperature and $\delta^{18}\mathrm{O_w}$:

$$\delta^{18}\mathrm{O_c} = -0.289T + 4.67 + \delta^{18}\mathrm{O_w}. \tag{S2.5}$$

Considering *changes* in a quantity X over glacial-interglacial cycles, i.e. $X_{(\mathrm{LIG})} - X_{(\mathrm{LGM})}$, then changes in Eq. S2.5 are:

$$\delta^{18}\mathrm{O_{c(LIG)}} - \delta^{18}\mathrm{O_{c(LGM)}} = -0.289(T_{(\mathrm{LIG})} - T_{(\mathrm{LGM})}) + \delta^{18}\mathrm{O_{w(LIG)}} - \delta^{18}\mathrm{O_{w(LGM)}}. \tag{S2.6}$$

Here, the linear relationship has the advantage that species-dependent offsets in $\delta^{18}\mathrm{O_c}$ due to vital effects (Rodríguez-Sanz et al., 2012) will cancel out.

The glacial-interglacial changes in seawater $\delta^{18}\mathrm{O_w}$ (i.e, $\delta^{18}\mathrm{O_{w(LIG)}} - \delta^{18}\mathrm{O_{w(LGM)}}$) were likely around 1‰ (Duplessy et al., 2002; Elderfield et al., 2010; de Boer et al., 2013). Meanwhile, glacial-interglacial temperature changes in Southern Ocean bottom waters were likely < 5°C (Elderfield et al., 2010; Hasenfratz et al., 2019). Therefore, according to Eq. S2.6, the glacial-interglacial bottom water temperature signal (less than 0.289×5‰)in benthic $\delta^{18}\mathrm{O_c}$ should have a similar or smaller magnitude when compared to the seawater $\delta^{18}\mathrm{O_w}$ signal (1‰).

Now turning to planktic $\delta^{18}\mathrm{O_c}$, if the glacial-interglacial amplitude of Southern Ocean SST changes is typically 4 to 8°C (see Results section of main text), then the SST signal in Eq. S2.6 is roughly 1 to 2‰, and is thus likely to be similar to or slightly greater than the seawater $\delta^{18}\mathrm{O_w}$ signal. Replacing the general −0.289‰/°C with specific coefficients for *G. bulloides* (-0.21‰/°C) or *N. pachyderma* (-0.27‰/°C) (Mulitza et al., 2003) reduces the magnitude of the SST signal only a little.

Fortunately, both the seawater isotopic and temperature signals tend to push $\delta^{18}O_c$ in the same direction, i.e., to lower (higher) values during interglacials (glacials). However, the influence of water temperature could still influence age models if maxima/minima in water temperature and $\delta^{18}O_w$ are not synchronous on millennial time scales. For benthic $\delta^{18}O_w$ we assume this influence of temperature is already accounted for in the regional $\delta^{18}O_c$ stacks described above (Lisiecki and Stern, 2016), especially when considering the relatively coarse (2 kyr) temporal resolution of the synthesis. However, we still need to consider how SST changes might affect the validity of using planktic $\delta^{18}O_c$ for age models.

S2.3 Validity of using planktic $\delta^{18}O_c$ in age models

To empirically evaluate the validity of using planktic $\delta^{18}O_c$ for age models in our study region, we examined six sites where both benthic and planktic $\delta^{18}O_c$ are available at reasonable resolution over the LIG (Fig. S2.2; see Table A1 in the main text for respective oxygen isotope and SST references). With only 6 suitable sites of very different temporal resolution, we limit our validation to a qualitative inspection. However, we note that this set of six sites includes at least one of each of the four relevant water masses in LS16 (DSA, DI, DP, IP). From inspection of Fig. S2.2, over the LIG we find that planktic $\delta^{18}O_c$ is likely to either (i) be synchronous with benthic $\delta^{18}O_c$ within the 2 kyr resolution, or (ii) lead benthic $\delta^{18}O_c$ by up to 5 kyr at the Events A and B shown in Fig. S2.1 .

In theory, the SST signal could be removed from the planktic $\delta^{18}O_c$ record using the reconstructed SST and paleotemperature equation (Eq. S2.1). In practice we do not do this, because the SST data themselves are noisy and subject to considerable uncertainty, as discussed in Section 2 of the main text (and also in Part 1). Overall, the use of planktic $\delta^{18}O_c$ may be considered to introduce an error reaching (exceptionally) $\sim$5 kyr in the age model. However, for most cases shown in Fig. S2.2, it is likely the resolution that dominates dating errors, rather than the use of planktic vs. benthic $\delta^{18}O_c$. Therefore, we do not find strong evidence against the use of planktic $\delta^{18}O_c$ for dating our records, given the relatively coarse 2 kyr time scale. We also note that an error of 5 kyr is within the differences (reaching 10 kyr) between age models established for the same sites by Capron et al. (2014) and Hoffman et al. (2017), as noted in Section 2.2 of the main text.

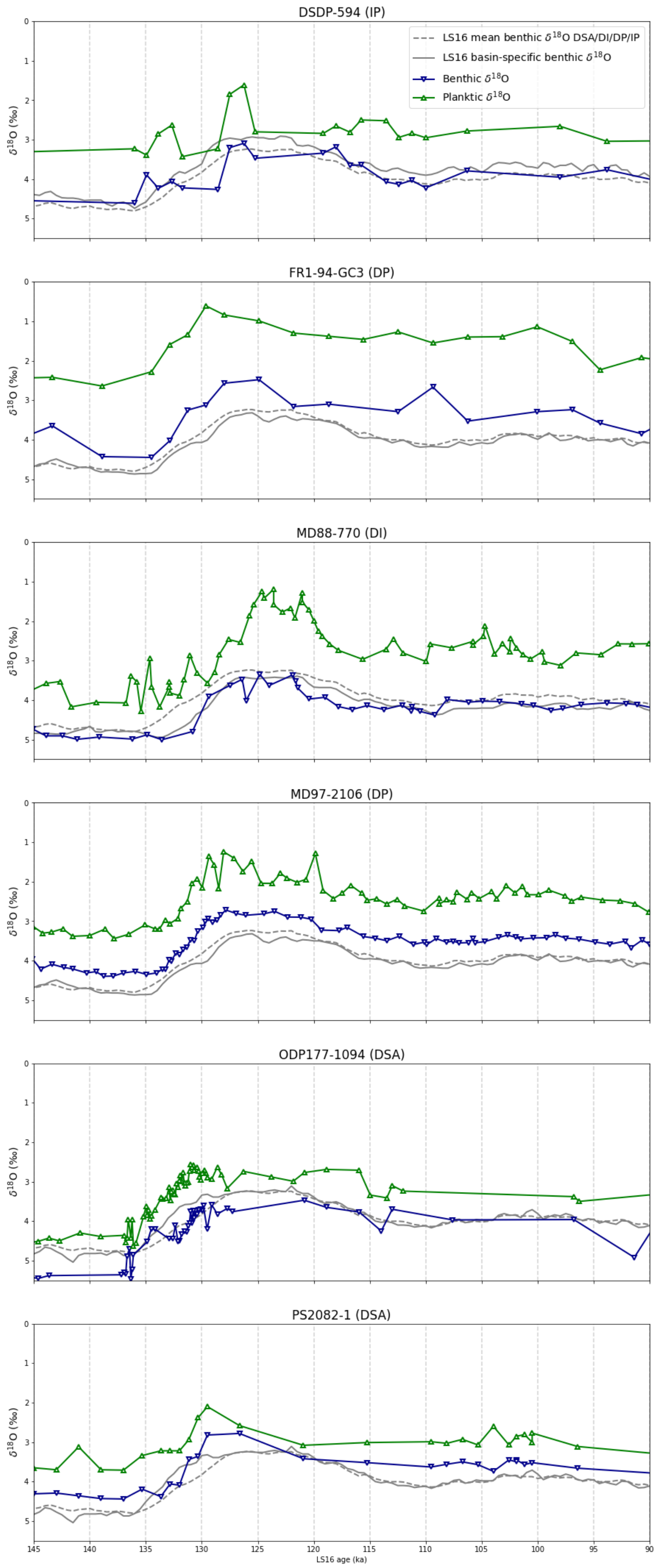

Figure S2.2: Foraminiferal $\delta^{18}O_c$ at sites where both planktic and benthic $\delta^{18}O_c$ data are available over the LIG. For site details see Table A1 in the main text. The grey lines are the LS16 basin-specific $\delta^{18}O_c$ stack (solid) and mean over the four relevant basins (DSA, DI, DP, IP: grey dashes).

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