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The cause of Late Cretaceous cooling: A multi-model/proxy comparison

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MODEL DESCRIPTIONS

CCSM4

We use the Community Climate System Model version 4 (CCSM4) maintained at the National Center for Atmospheric Research (NCAR). Our model component-set includes the Community Atmospheric Model version 4 (CAM4), the Community Land Model version 4 with dynamic vegetation (CLM4-DGVM), the Parallel Ocean Project model version 2 (POP2), and the Community Sea Ice model version 4 (CICE4). Additional details on the model components and performance can be found in Gent et al. (2011), and information on the DGVM is

documented in Levis et al. (2004). The ocean and sea ice models run on a rotated poles grid at roughly 1° resolution with 60 vertical ocean levels. The atmosphere and land-surface models run on a finite-volume grid of 1.9×2.5°, and the atmosphere has 28 vertical levels. We run CAM4 with the Bulk Aerosol Model (BAM), a prognostic aerosol model, with aerosol concentrations and types adjusted for the Cretaceous using a method similar to Heavens et al. (2012). Here, aerosol data come from pre-industrial datasets converted into hemispherically symmetric, monthly zonal average aerosols distributions masked independently to land and sea. In addition, we add the land black carbon emissions from 62.5°N/S to all latitudes further poleward to reflect the greater vegetation cover and fire potential at high latitudes during the Cretaceous (Upchurch et al., 1998). We run all simulations for 1500 years with all model components active and synchronously coupled.

HadCM3L

We also use the Hadley Centre Model (HadCM), developed by the UK Met Office. For this study, we implement HadCM3L version 4.5, which contains dynamic atmosphere, ocean, land, and sea ice components on a 2.5×3.75° grid. The ocean and atmosphere have 19 and 20 vertical levels, respectively. Description of the similar HadCM3 model is documented in Gordon et al. (Gordon et al., 2000). We couple HadCM3L with the Top-down Representation of Interactive Foliage and Flora Including Dynamics (TRIFFID) model with the land surface scheme MOSES 2.1 to simulate dynamic vegetation (Cox, 2001). We run the HadCM3 experiments in 4 phases:

1. 50 years with 280 ppm CO₂ and bare-ground

2. 319 years of either 560 or 1120 ppm CO₂ with TRIFFID turned on
3. 53 years with the addition of prescribed lakes
4. 1000 years with barotropic ocean flow enabled to allow non-zero vertically integrated ocean flow

For additional details on HadCM3L initialization and spin-up see Lunt et al. (2015).

MODELS SETUP

Simulations use the paleogeographic reconstructions of Gedge Plc. Following model standard practices and for improved stability, we apply model specific smoothing to the topography. For both models, we adjust total TSI for the Cenomanian (CEN) and Maastrichtian (MAA) based on the equation of Gough (1981). We prescribe CO₂ concentrations as either 4x (1120 ppm) or 2x preindustrial (560 ppm). All other GHG concentrations are set to preindustrial values of 790 ppb for CH₄, 275 ppb for N₂O, and no CFCs. The orbit configuration is set to present-day. Vegetation plant functional types are model defaults; we make no adjustments for the Cretaceous. All simulations run long enough for the upper ocean to reach near-equilibrium; however, the deep ocean continues to adjust. As a result, we focus only on surface conditions.

ENERGY BALANCE CALCULATIONS

We use the zonal mean energy balance decomposition method of Heinemann (2009), which was subsequently adopted and modified by Lunt et al. (2012), and Hill et al. (2014), to explore the mechanisms responsible for surface temperature change in the Late Cretaceous with changes in paleogeography and CO₂. This method assumes incoming shortwave balances with outgoing longwave and that local imbalances are due to changes heat convergence, using the

following relationship:

$$\frac{S_0}{4}(1 - \alpha) + H = \varepsilon \sigma T^4 . (1)$$

Here, S_0 is TSI, α is albedo, H is meridional heat convergence, ε is emissivity, σ ($5.67 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4}$) is the Stefan-Boltzmann constant, and T is surface temperature. With the exception of σ , values in equation (1) come from zonal averages of Earth system model outputs. We can rewrite equation (1) with respect to surface temperature as:

$$T = \left(\frac{1}{\varepsilon \sigma} \left(\frac{S_0}{4}(1 - \alpha) + H \right) \right)^{0.25} \equiv E(\varepsilon, \alpha, H) . (2)$$

By substituting variables from different simulations and differencing them, we can deconstruct the various contributions to the change in surface temperature. We illustrate this below:

$$\Delta T_{emm} = E(\varepsilon, \alpha, H) - E(\varepsilon', \alpha, H) . (3)$$

$$\Delta T_{alb} = E(\varepsilon, \alpha, H) - E(\varepsilon, \alpha', H) . (4)$$

$$\Delta T_{tran} = E(\varepsilon, \alpha, H) - E(\varepsilon, \alpha, H') . (5)$$

where ΔT_{emm} , ΔT_{alb} , and ΔT_{tran} are contributions from emissivity, albedo, and heat convergence to surface temperature change, and primes represent the zonal averages from the simulations being compared. The combination of surface temperature changes due to emissivity, albedo, and heat convergence sum to approximate the total surface temperature response:

$$\Delta T_{total} \cong \Delta T_{emm} + \Delta T_{alb} + \Delta T_{tran} . (6)$$

This technique can be used to further decompose the climate contributions to surface temperature.

PROXY DATA

As mentioned in the main text, SST proxy values represent location and age averages. Method uncertainties only accounts for calibration uncertainties. We apply these uncertainties to every averaged data point. The range in values from a particular age and site are often significantly greater than the calibration uncertainties. Therefore, uncertainties represent minimum estimates.

Point locations are consistently rotated back in time from their present-day sampling locations to the CEN and MAA using the plate reconstructions from Getech Plc. Occasionally, the coarse model resolutions result in marine proxy paleo-locations over land instead of water. In these situations, we select the nearest model ocean location to represent the SST value.

To create more representative latitudinal SST gradients, Gaussian fits of the proxies include an adjustment for the deviation of the SSTs from the zonal mean based on model-simulated longitudinal heterogeneity. For example, if an equatorial proxy location has a model simulated SST of 30°C and a model zonal mean equatorial SST of 35°C, then 5°C are added to the proxy value so that it is in better agreement with the zonal average. This technique assumes that model longitudinal variability is robust regardless of mean SSTs.

We investigate the statistical similarity between the temperature gradients of our CEN and MAA datasets using an F-test. An F-test determines if the variance of multiple datasets are statistically different from each other. To standardize the data, we first remove the global means of the Gaussian fitting procedure (Fig. 2d). Then, we apply an F-test to test the hypothesis that the spread of residual SSTs between the CEN and MAA are statistically distinct. Our results produce a p-value equal to 0.39, which suggests that SST variations, except for the means

between datasets, are not robust.

Seawater $\delta^{18}\text{O}$

We assume a mean $\delta^{18}\text{O}_{\text{sw}}$ of -1^0_{00} VSMOW, based on the assumption of an ice-free world (Shackleton and Kennett, 1975). This assumption is widely used in Cretaceous SST reconstructions (e.g. Huber et al., 2002; Friedrich et al., 2012); however, debate remains about the potential for glaciation in the Late Cretaceous (e.g. Miller et al., 2005). A significant increase in land-ice would require less cooling in the MAA from $\delta^{18}\text{O}$ records but is not considered further in this study.

$\delta^{18}\text{O}_{\text{sw}}$ has significant regional variability in both the modern and Late Cretaceous (Zhou et al., 2008). To account for this variability, we use zonal average salinity from the model outputs with the present-day salinity/ $\delta^{18}\text{O}_{\text{sw}}$ relationship of Broecker (1989). This simple linear relationship follows:

$$\delta^{18}\text{O}_{\text{w}} = 0.5(PSU) - 17.12 . (7)$$

where *PSU* stands for positive salinity units. In our simulations, mean ocean salinity starts at 35 PSU, which is equivalent to present-day. While not perfect, we prefer this relationship to the commonly employed present-day latitudinal $\delta^{18}\text{O}_{\text{sw}}$ correction by Zachos et al. (1994), because it indirectly accounts for precipitation and evaporation, and does not make present-day assumptions about the latitudinal distribution of $\delta^{18}\text{O}_{\text{sw}}$ (Poulsen et al., 1999). Still, this technique is inferior to model experiments that include water isotope tracking (e.g. Zhou et al., 2008).

Planktonic Foraminifera

We calculate SSTs from $\delta^{18}\text{O}$ measurements of planktonic foraminifera using the calibration of Erez and Luz (1983) and a conversion to VSMOW of -0.22‰ (Bemis et al., 1998). This calibration has been widely used for foraminifera temperature reconstructions and proven accurate for a wide range of temperatures. Temperatures are calculated using the polynomial:

$$T(^{\circ}\text{C}) = 16.998 - 4.52[\delta^{18}\text{O}_c - \delta^{18}\text{O}_{sw}] + 0.028[\delta^{18}\text{O}_c - \delta^{18}\text{O}_{sw}]^2 . \quad (8)$$

where $\delta^{18}\text{O}_c$ is the $\delta^{18}\text{O}$ of sample calcite.

Diagenetic alteration is a potential issue for foraminifera, causing them to pickup post-depositional temperature signals from the ocean floor (e.g. Pearson et al., 2001; Norris et al., 2002). It is likely that some of the foraminifera presented in this study suffer from such alteration given the sample descriptions, relatively cool tropical SSTs, and disagreement with other SST proxy values. However, given the paucity of records and uncertainty in other included proxy techniques such as TEX_{86} (e.g. Taylor et al., 2013), we opt to include all planktonic foraminifera data. For comparison, we include zonal SST reconstructions without foraminifera as well (Fig. DR8, DR9, DR10). Even though removal of foraminifera leads to warmer tropical SST reconstructions, it does not significantly change the magnitude of cooling from the CEN to the Maa, which is the main focus of this study. We assign an uncertainty of $\pm 2.9^{\circ}\text{C}$ for planktonic foraminifera based on Holocene core-top data from Crowley and Zachos (Crowley and Zachos, 2000) and to be consistent with the work of Upchurch (2015).

Shells and Others

We use the $\delta^{18}\text{O}$ to temperature conversion of Anderson and Arthur (1983) for both

aragonite and calcite of shells of mollusks, bivalves, brachiopods, and belemnite rostra based on its prevalent use in the proxy source literature (Grossman, 2012). The equation is:

$$T(^{\circ}C) = 16.4 - 4.14(\delta^{18}O_{c/a} - \delta^{18}O_{sw}) + 0.13(\delta^{18}O_{c/a} - \delta^{18}O_{sw})^2 . (9)$$

where $\delta^{18}O_{c/a}$ is the $\delta^{18}O$ of sample calcite or aragonite. Like foraminifera, shells are prone to alteration (Steuber et al., 1999). We include all records here for completeness. We also show comparisons with shell SST proxies omitted (Fig. DR8, DR9, DR10). We apply an uncertainty of ± 1.6 based on 1σ of a mollusk calibration by Grossman and Ku (1986) as in Upchurch et al. (2015).

Tooth Enamel $\delta^{18}O$

Our SST proxy compilation includes phosphate $\delta^{18}O$ records from fish tooth enamel, most of which were originally compiled by Puc  at et al. (2007). These records are considered more resistant to diagenetic alteration than foraminifera or shells, and were previously used by Puc  at et al. (2007) to argue for a near-modern latitudinal SST gradient in the Cretaceous, in contrast to reconstructions from foraminifera that suggested a shallower latitudinal SST gradient (e.g. Huber et al., 2002). Recently, there have been several recalibrations of the phosphate $\delta^{18}O$ temperature relationship. Here, we use the most recent calibration by Lecuyer et al. (2013):

$$T(^{\circ}C) = 117.4 - 4.5(\delta^{18}O_{PO_4} - \delta^{18}O_{sw}) . (10)$$

where $\delta^{18}O_{PO_4}$ is the $\delta^{18}O$ of sample phosphate. This calibration results in SSTs that are several degrees warmer than the calibration by Puc  at et al. (2007) and several degrees cooler than the recent calibration by Puc  at et al. (2010). However, the magnitude of offset between calibrations remains quite similar over the range of $\delta^{18}O_{PO_4}$ values. Therefore, while the absolute temperature

reconstructions differ depending on the chosen calibration, the difference between the CEN and MAA records is small. In addition, the calibration of Lecuyer et al. (2013) benefits from the smallest uncertainty of $\pm 1.2^{\circ}\text{C}$, which we apply to all tooth enamel SST values.

TEX₈₆

TEX₈₆ is a relatively new SST proxy method based on the ratio of different glycerol dialkyl glycerol tetraethers (GDGTs) with 86 carbons, which comprise membrane lipids in marine Crenarchaeota (Schouten et al., 2002). It has the benefit of not relying on $\delta^{18}\text{O}_{\text{sw}}$ assumptions. Here, we use the calibration of Kim et al. (2010) TEX₈₆^H, which provides the smallest error in warm climate conditions. The equation is:

$$T(^{\circ}\text{C}) = 68.4 \log(\text{TEX}_{86}) + 38.6 . \quad (11)$$

Modern calibration by Kim et al. (2010) show an uncertainty of $\pm 2.5^{\circ}\text{C}$, which we use in our model/proxy comparison.

We include the high-latitude MAA TEX₈₆^H SST value from Jenkyns et al. (2004) in our tables and plots for reference but do not include it in our analyses. We find, like several former studies (Davies et al., 2009; Spicer and Herman, 2010; Upchurch et al., 2015), that this value represents an extreme outlier from other proxy data and model results. Inclusion of this data point significantly skews our results, because it is the only available Arctic MAA SST value. Based on our other findings, it requires roughly 10°C warming from 50°N to 80°N , for which we have no physical basis.

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Figure DR1. Getech Plc CEN and MAA paleogeography with marine proxy locations.

Figure DR2: Individual model simulated Late Cretaceous mean annual surface temperatures and temperature responses to changes in paleogeography and CO₂ concentration. Row 1 shows CCSM4 mean annual surface temperatures from CEN4x (A), MAA4x (B), and MAA2x (C). Row 2 shows HadCM3L mean annual surface temperatures from CEN4x (D), MAA4x (E), and MAA2x (F). Row 3 shows CCSM4 mean annual surface temperature differences between CEN4x and MAA4x (G), MAA4x and MAA2x (H), and CEN4x and MAA2x (I). Row 4 shows HadCM3L mean annual surface temperature differences between CEN4x and MAA4x (J), MAA4x and MAA2x (K), and CEN4x and MAA2x (L). The large-scale surface temperature patterns are quite similar for both models.

Figure DR3. Late Cretaceous mean annual total cloud cover and anomalies. Column 1 shows the model total cloud cover from A) CEN4x, B) MAA4x, and C) MAA2x. Column 2 shows the difference in total cloud cover between D) CEN4x and MAA4x, E) MAA4x and MAA2x, and F) CEN4x and MAA2x. Column 3 shows the total cloud cover anomalies between CCSM4 and HadCM3L for G) CEN4x, H) MAA4x, and I) MAA2x. Clouds remain one of the largest uncertainties in climate models. Both models show similar cloud patterns for all model configurations. However, the range of cloud cover between regions is more pronounced in HadCM3L than CCSM4. The configuration of the CCSM4 aerosols for paleoclimate might be partly responsible for the discrepancies in cloud magnitude.

Figure DR4. Late Cretaceous mean annual surface albedo and anomalies. Column 1 shows the model surface albedo from A) CEN4x, B) MAA4x, and C) MAA2x. Column 2 shows the difference in surface albedo between D) CEN4x and MAA4x, E) MAA4x and MAA2x, and F)

209 CEN4x and MAA2x. Column 3 shows the surface albedo anomalies between CCSM4 and
 210 HadCM3L for G) CEN4x, H) MAA4x, and I) MAA2x. In the high-latitudes, CCSM4 simulates
 211 higher surface albedos than HadCM3L due to differences in sea ice cover and vegetation.
 212 CCSM4 tends to produce more sea in the Arctic than HadCM3L, which leads to greater
 213 shortwave reflection, especially in the spring and fall. CCSM4 also grows shorter, less dense
 214 vegetation than HadCM3L in the polar regions. A lower vegetation and reduced canopy allows
 215 for more snow cover of vegetation, which raises the albedo. Tall, dense Antarctic vegetation
 216 suggested by paleobotanical reconstructions is not simulated in CCSM4 (e.g. Upchurch et al.,
 217 1998). Modification of the vegetation model will be an important step in our future work, as
 218 some research shows vegetation can help remedy model/proxy LST discrepancies (e.g. Otto-
 219 Bliesner and Upchurch, 1998; Zhou et al., 2012).
 220 Figure DR5. Zonal mean annual SST responses to changing topography and decreasing CO₂ for
 221 both CCSM4 and HadCM3L models. Comparison of CCSM4 and HadCM3L outputs highlight
 222 the similarities in surface temperature response.
 223 Figure DR6. Decomposition of the simulated changes in zonal mean surface temperature into
 224 contributions from heat convergence (red), emissivity (green), albedo (blue), and TSI (yellow)
 225 for A) CCSM4 and B) HadCM3L changes in geography, C) CCSM4 and D) HadCM3L changes
 226 in CO₂, and E) CCSM4 and F) HadCM3L changes in both geography and CO₂. See Data
 227 Repository for details on energy balance calculations.
 228 Figure DR7. Seasonal sea ice exists in all 4x PI CO₂ simulations in agreement with some proxies
 229 that find evidence for Arctic sea ice during peak Cretaceous warmth (Davies et al., 2009). The

Arctic experiences an increase in sea ice concentration from the CEN to MAA because the Arctic becomes more restricted in the Maa. With a reduction in CO₂, a significant amount of perennial sea ice forms in the Arctic while Antarctic sea ice remains mostly seasonal. This contrast in sea ice between hemispheres is similar to present-day where the restricted Arctic promotes retention of sea ice, and the open ocean Antarctic allows the equator drift and wasting of sea ice.

In all experiments, CCSM4 produces greater Arctic sea ice cover and less Antarctic sea ice cover than HadCM3L. This contrast relates to the differences in open ocean SSTs between models. In general, CCSM4 has greater ocean overturning in the high Southern latitudes, which promotes transports of warm equatorial water poleward and inhibits sea ice formation. In contrast, there is less deep-water formation in the high Northern latitudes in either model.

Further, the Late Cretaceous Arctic is quite restricted from the greater ocean, especially in the Maa, which prevents warm open ocean waters from having a large effect.

Figure DR8. Latitudinal temperature gradient reconstructions from the CEN with the systematic removal of SST proxy reconstruction data from individual methods. Simulated CEN4x zonal average SSTs with all CEN proxies SST except A) foraminifera, B) fish tooth enamel, C) shells and related structures, and D) TEX₈₆. Removal of foraminifera leads to a significantly warmer equator and steeper equator-to-pole temperature gradient. This gradient is steeper than model simulated SSTs. It appears likely that some foraminifera are not recording a pure SST signal.

Figure DR9. Latitudinal temperature gradient reconstructions from the MAA with the systematic removal of SST proxy reconstruction data from individual methods. Simulated MAA4x zonal

average SSTs with all MAA proxies SST except A) foraminifera, B) fish tooth enamel, C) shells and related structures, and D) TEX₈₆. Like for the Cen, removal of foraminifera leads to a significantly warmer equator and steeper equator-to-pole temperature gradient.

Figure DR10. Identical to figure S7 except with simulated MAA2x data plotted.

Figure DR11. SST model/proxy discrepancies by latitude. A) Differences between CEN proxies and CEN4x simulations. B) Differences between MAA proxies and MAA4x simulations. C) Differences between MAA proxies and MAA2x simulations. In general, the CEN4x simulations have a cold bias while the MAA4x simulations have a warm bias. The MAA2x simulations are in better agreement with SST proxies. A model warm bias remains in the equatorial region in the MAA2x, but this might be a result of diagenetic alteration of planktonic foramina. While beyond the scope of this work, calibration choices also impact model/proxy agreement. For example, the warmer fish tooth enamel calibration of Puc  at et al. (2010) might result in a better agreement between models and proxies for the MAA2x simulations.

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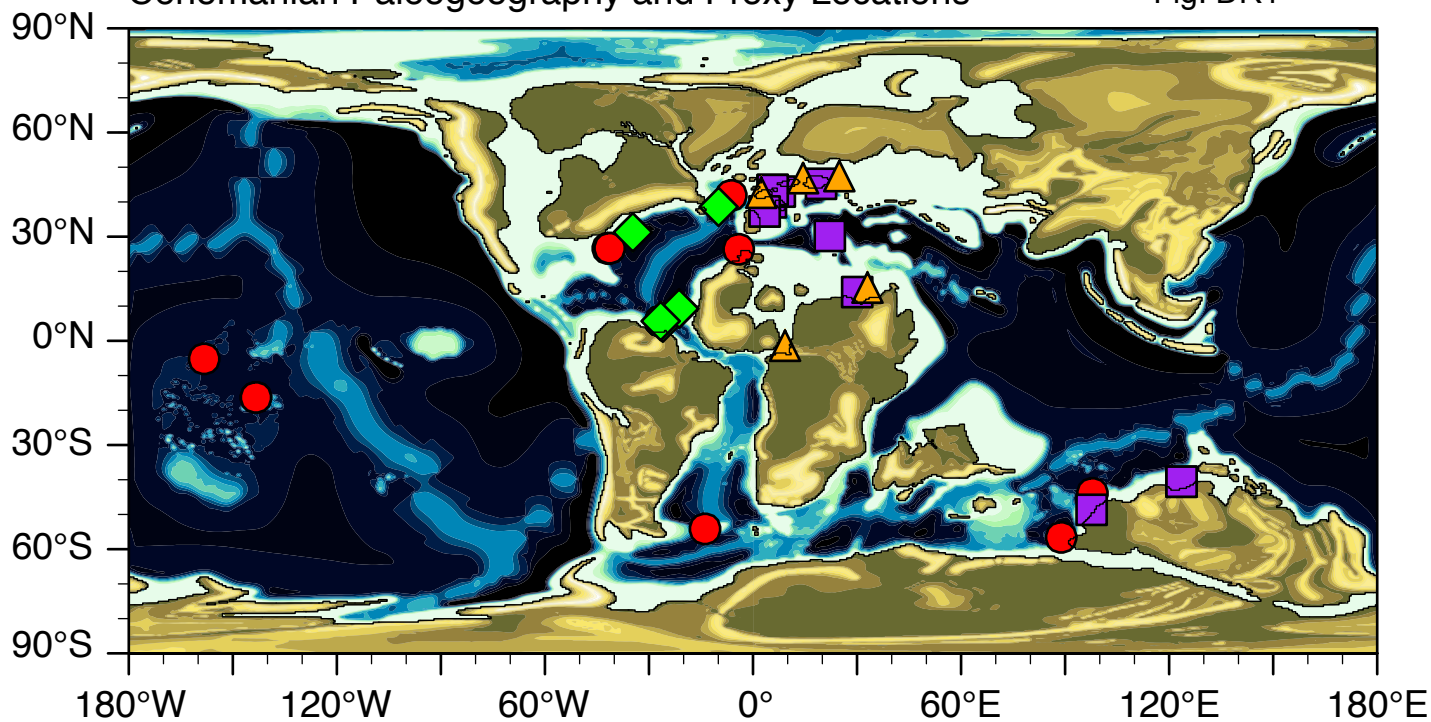
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Cenomanian Paleogeography and Proxy Locations

Fig. DR1



Maastrichtian Paleogeography and Proxy Locations

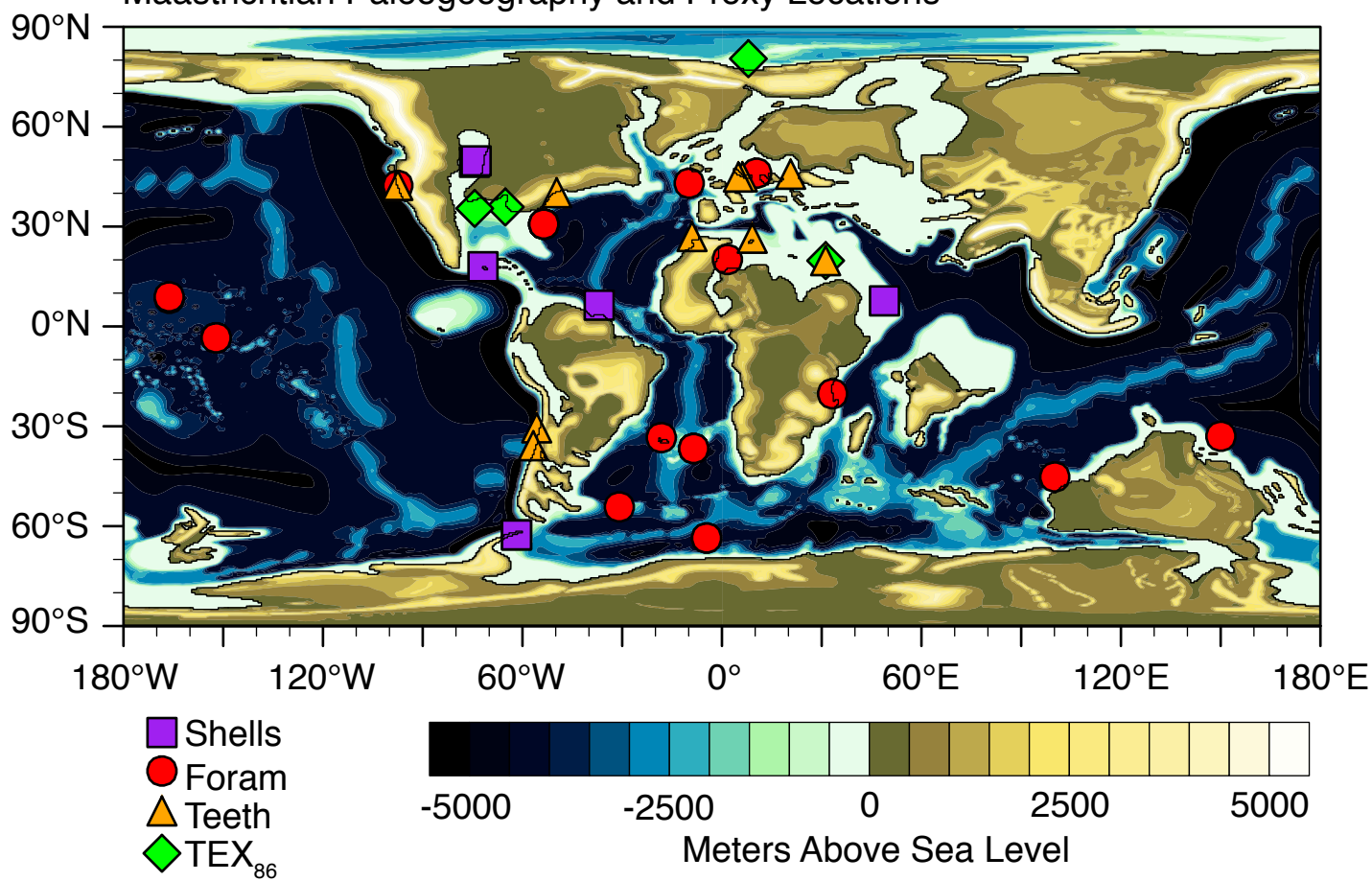
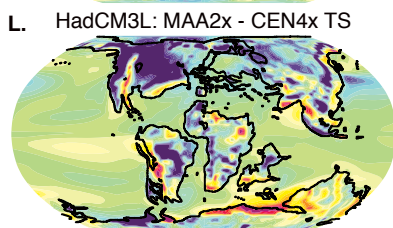
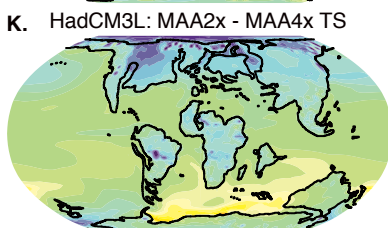
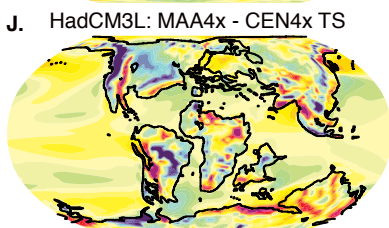
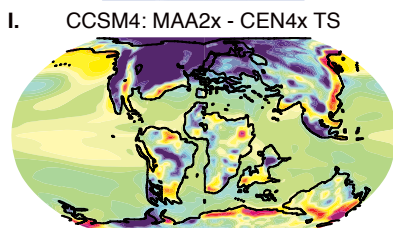
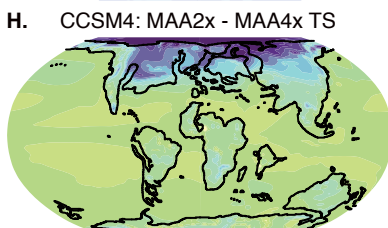
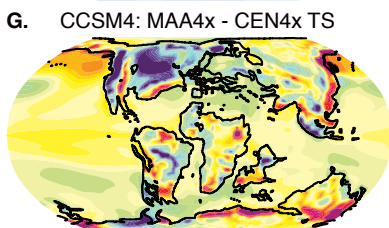
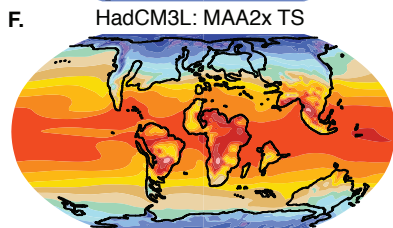
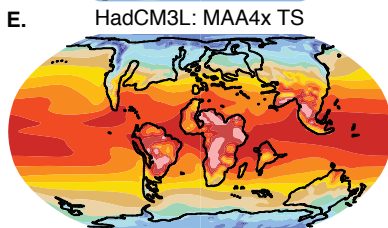
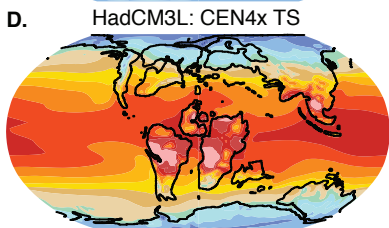
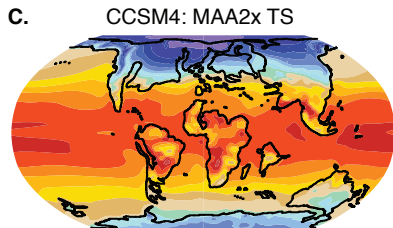
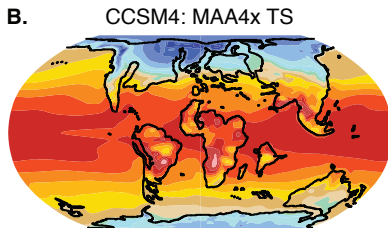
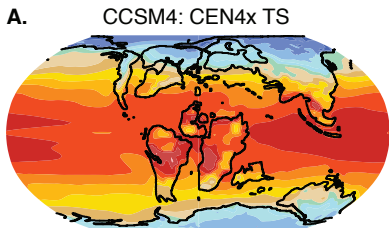
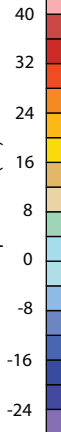


Fig. DR2

Temperature (°C)



Temperature (°C)

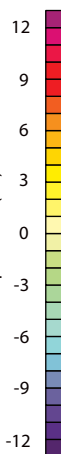


Fig. DR3

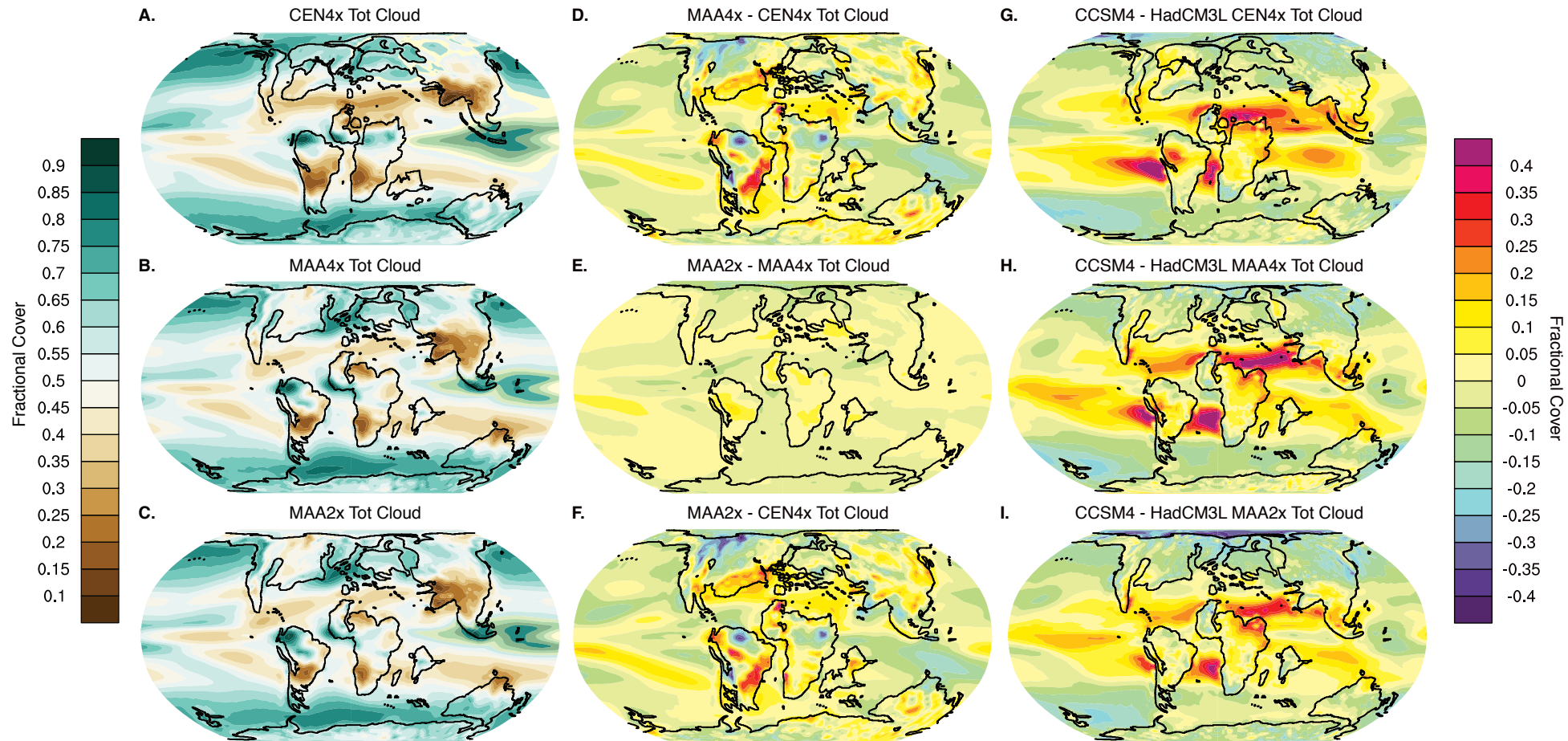
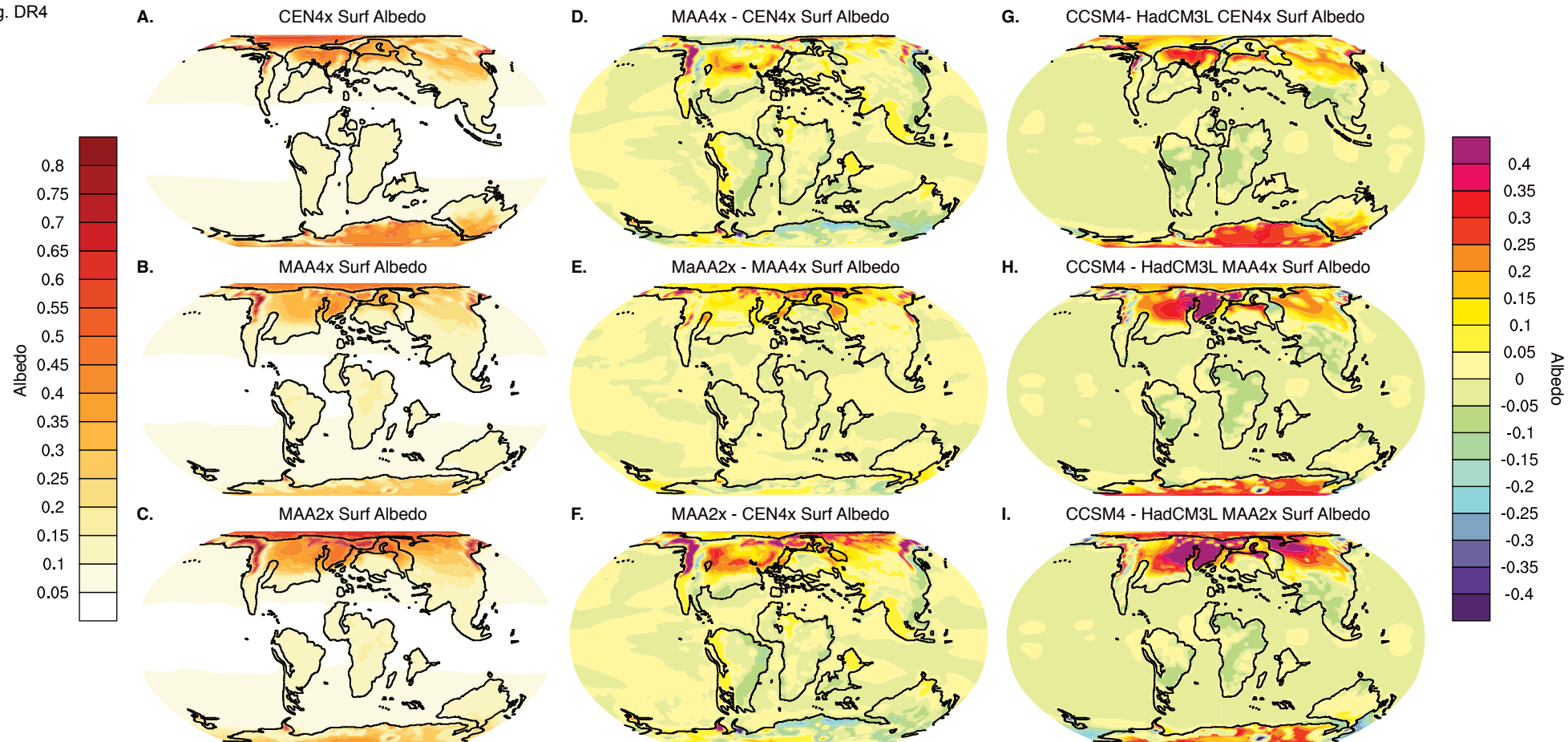


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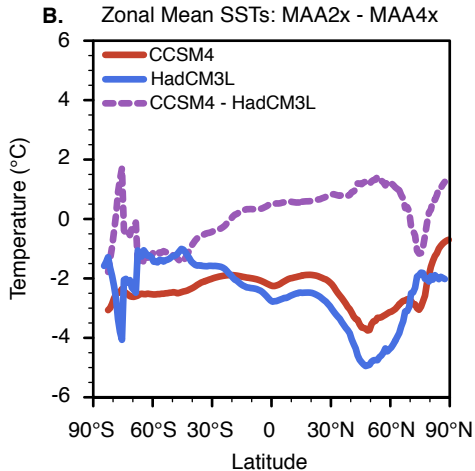
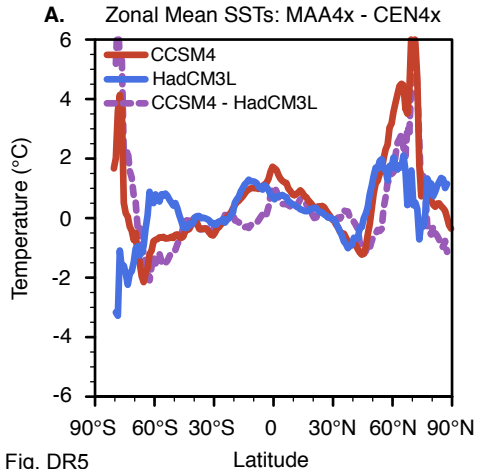


Fig. DR5

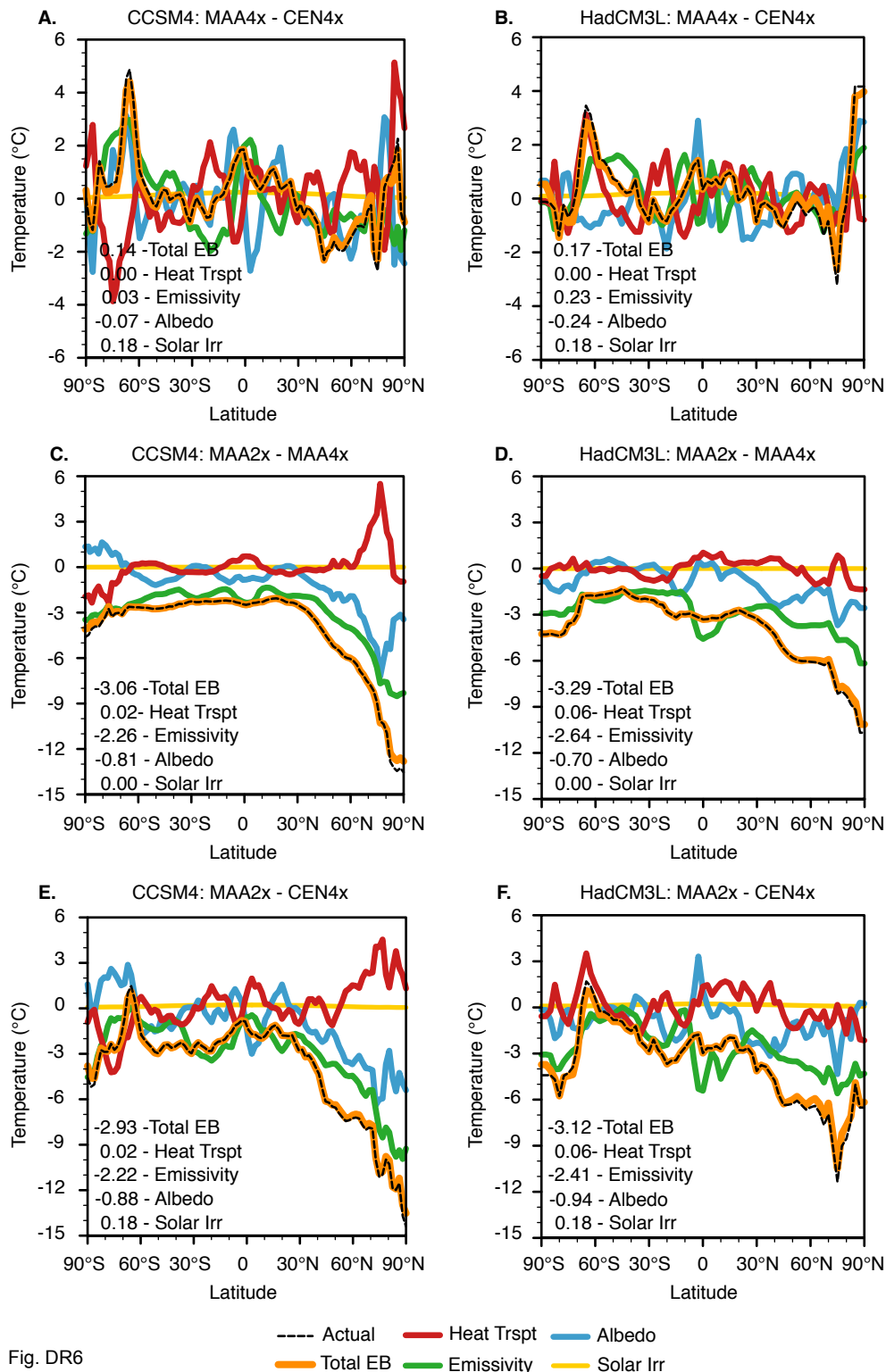
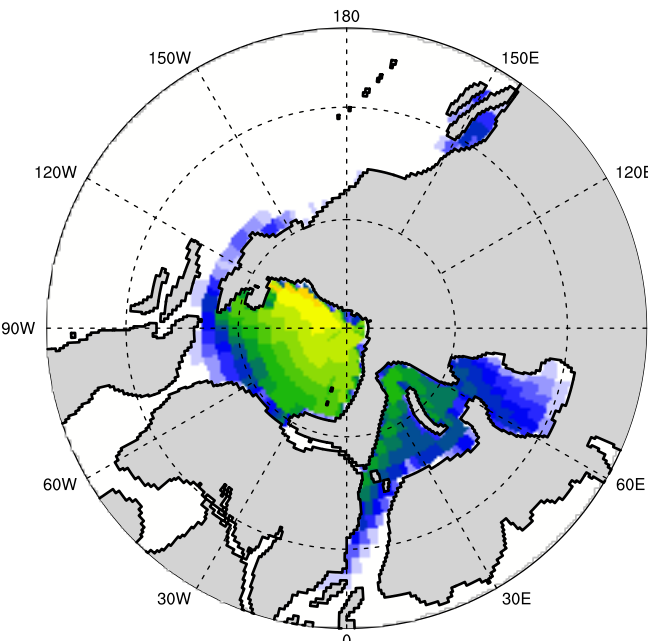
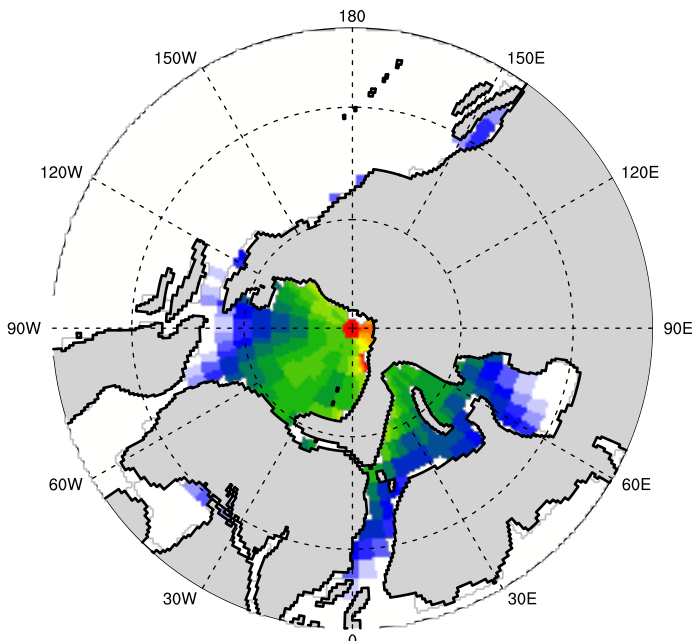


Fig. DR6

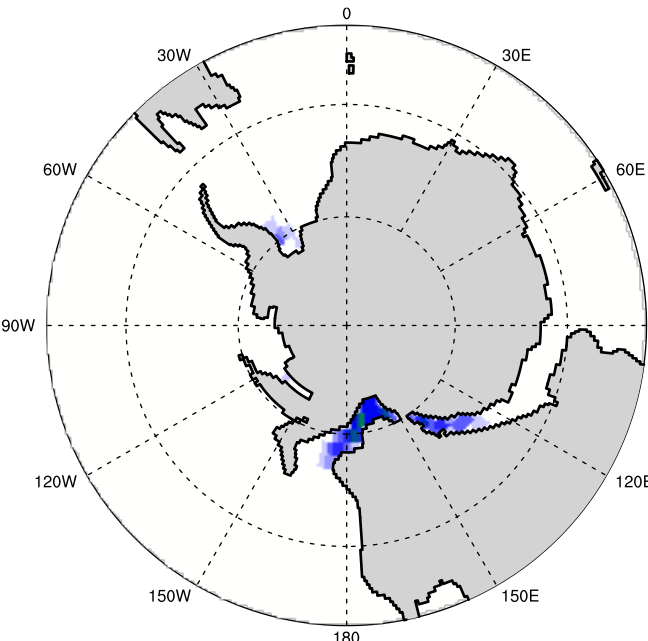
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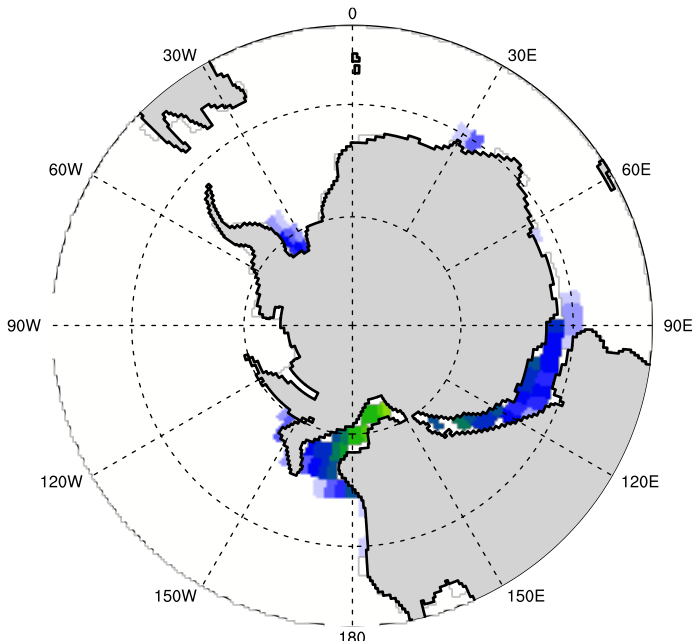
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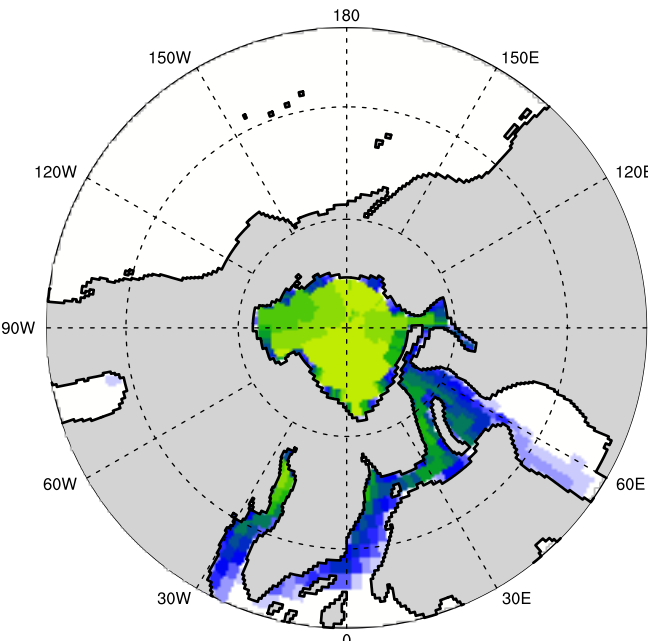
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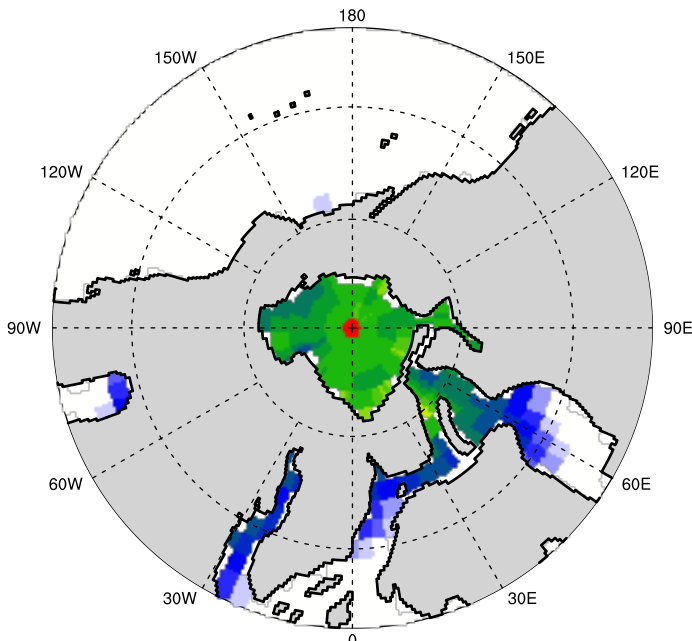
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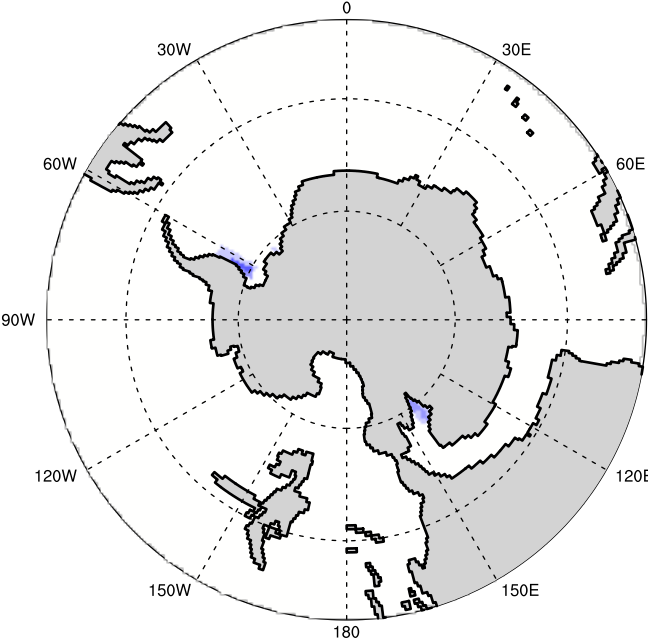
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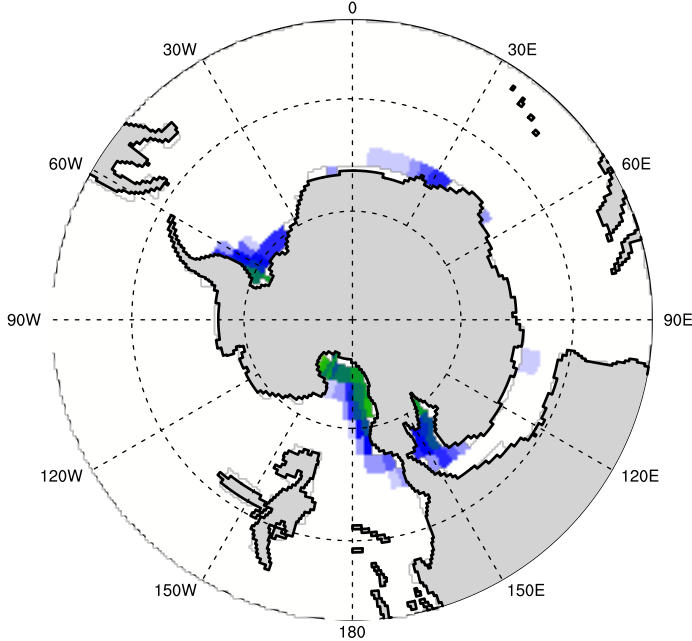
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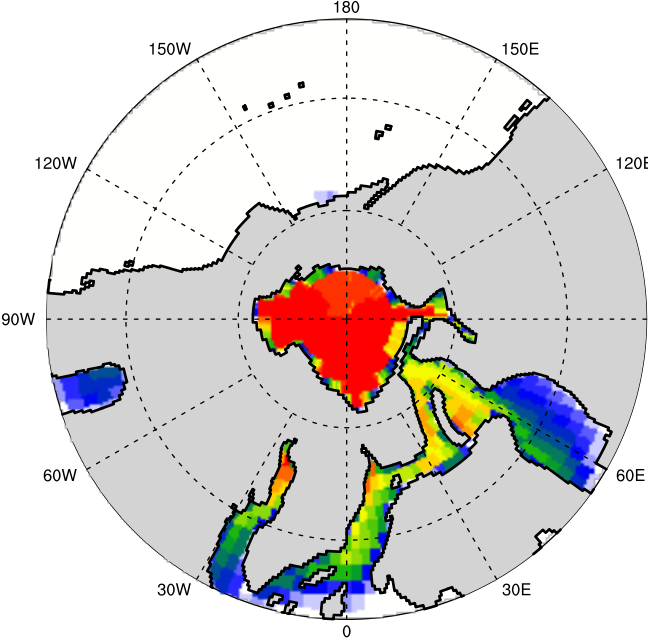
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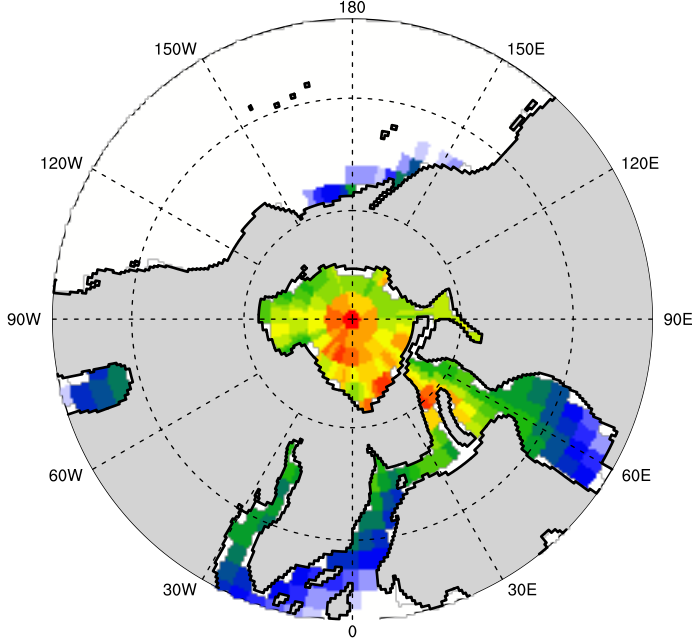
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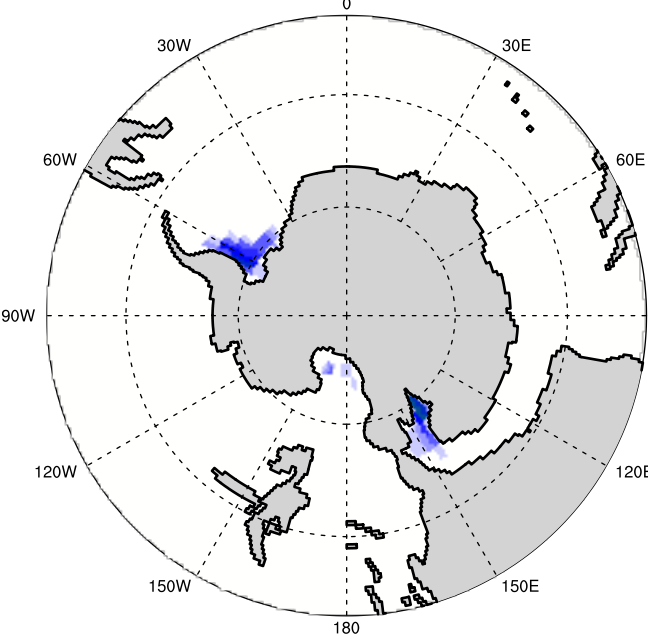
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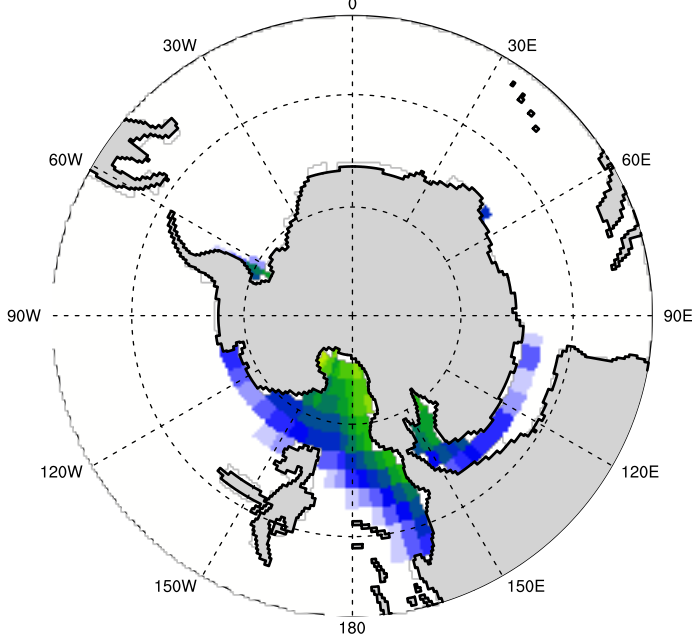
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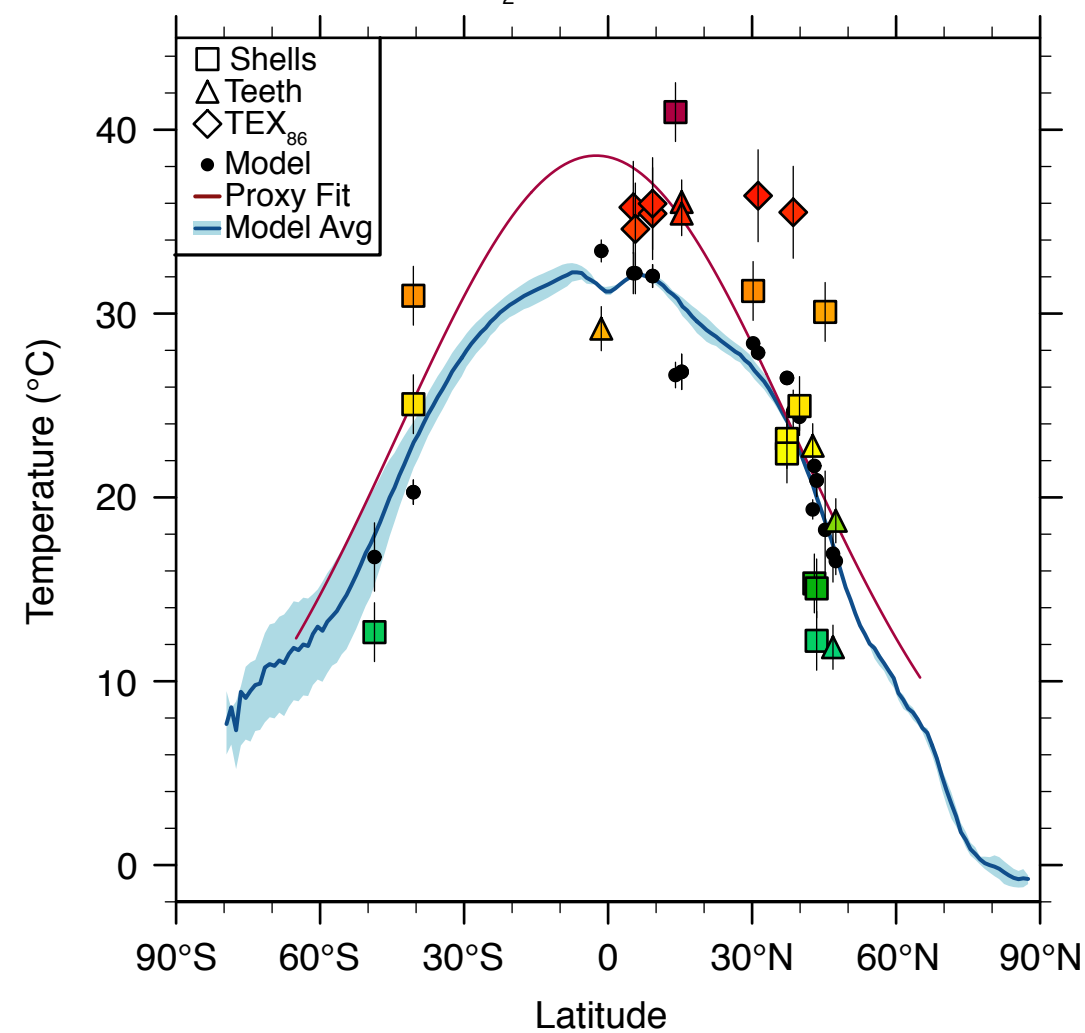
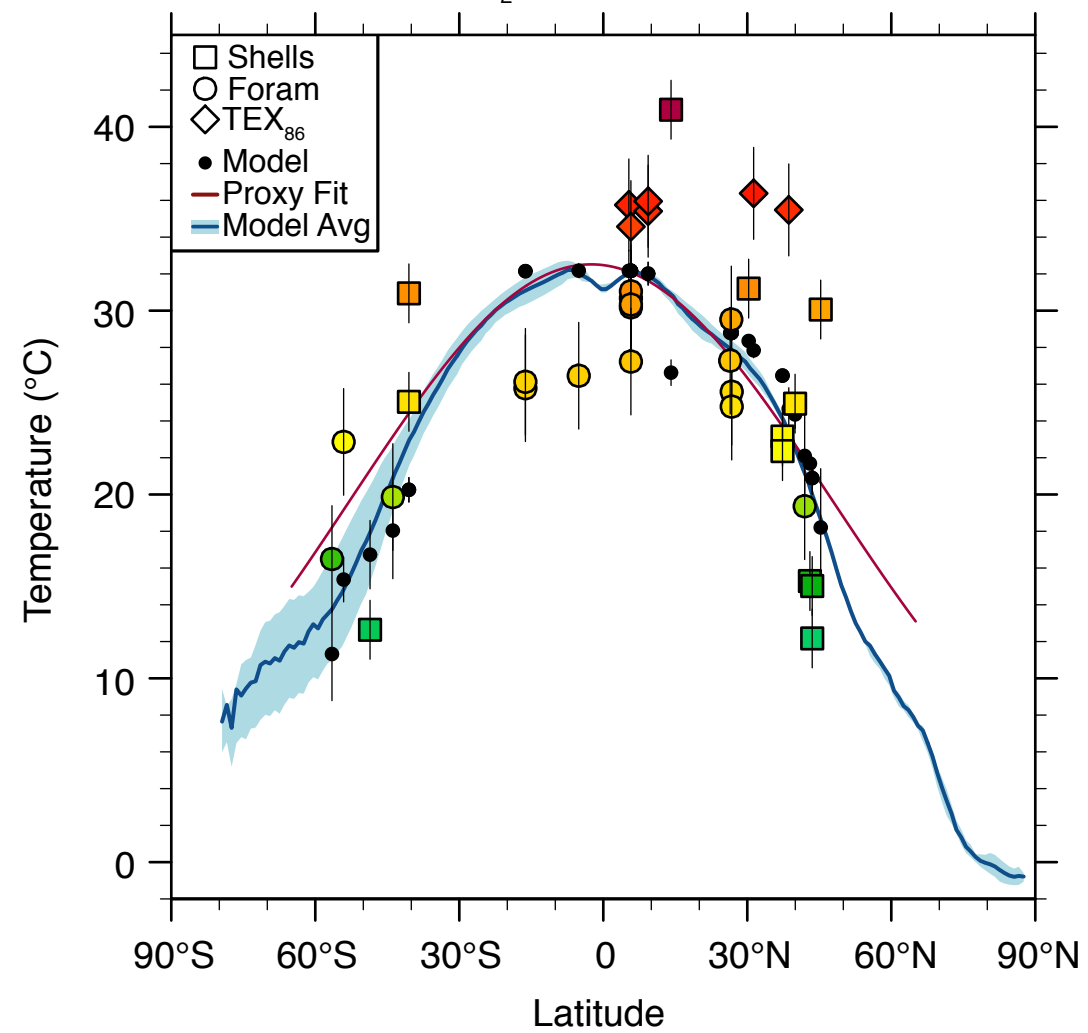
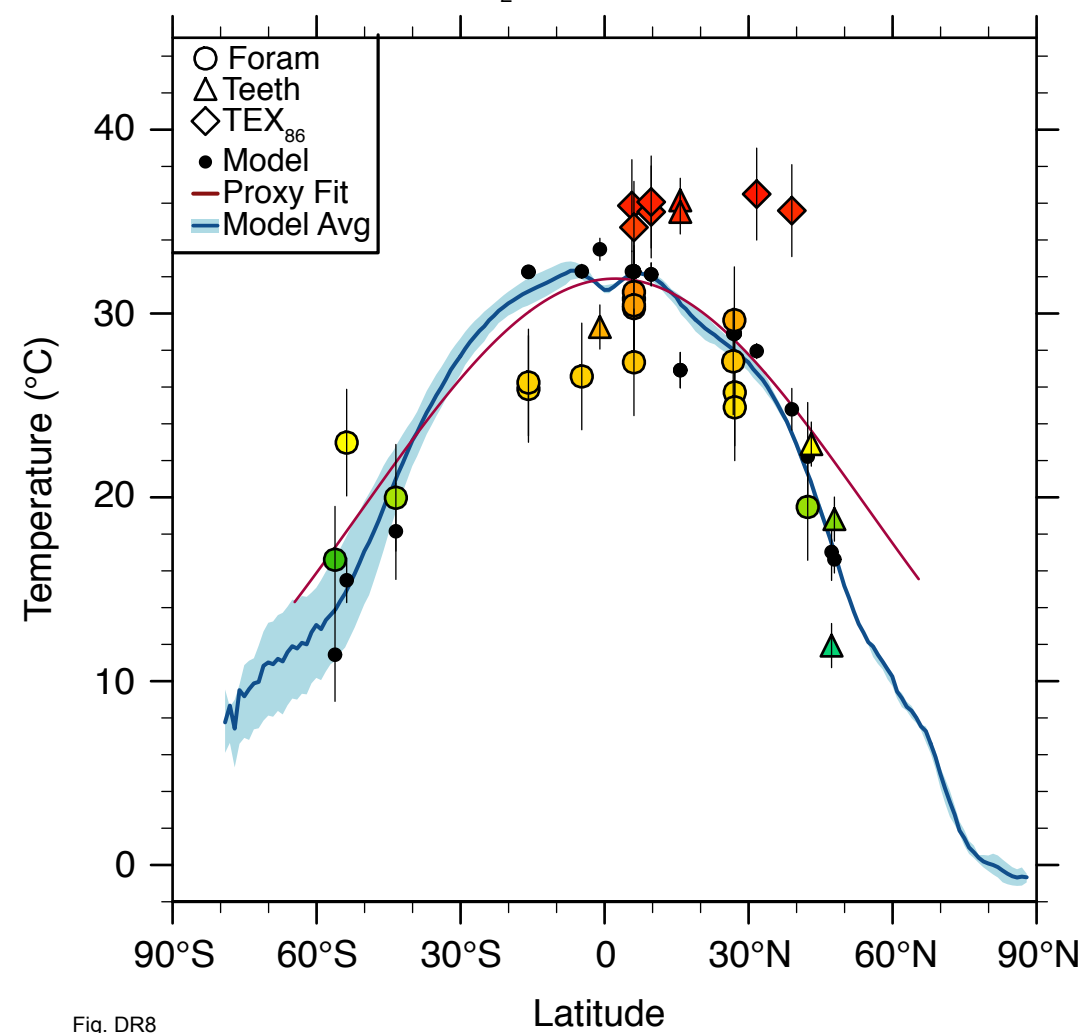
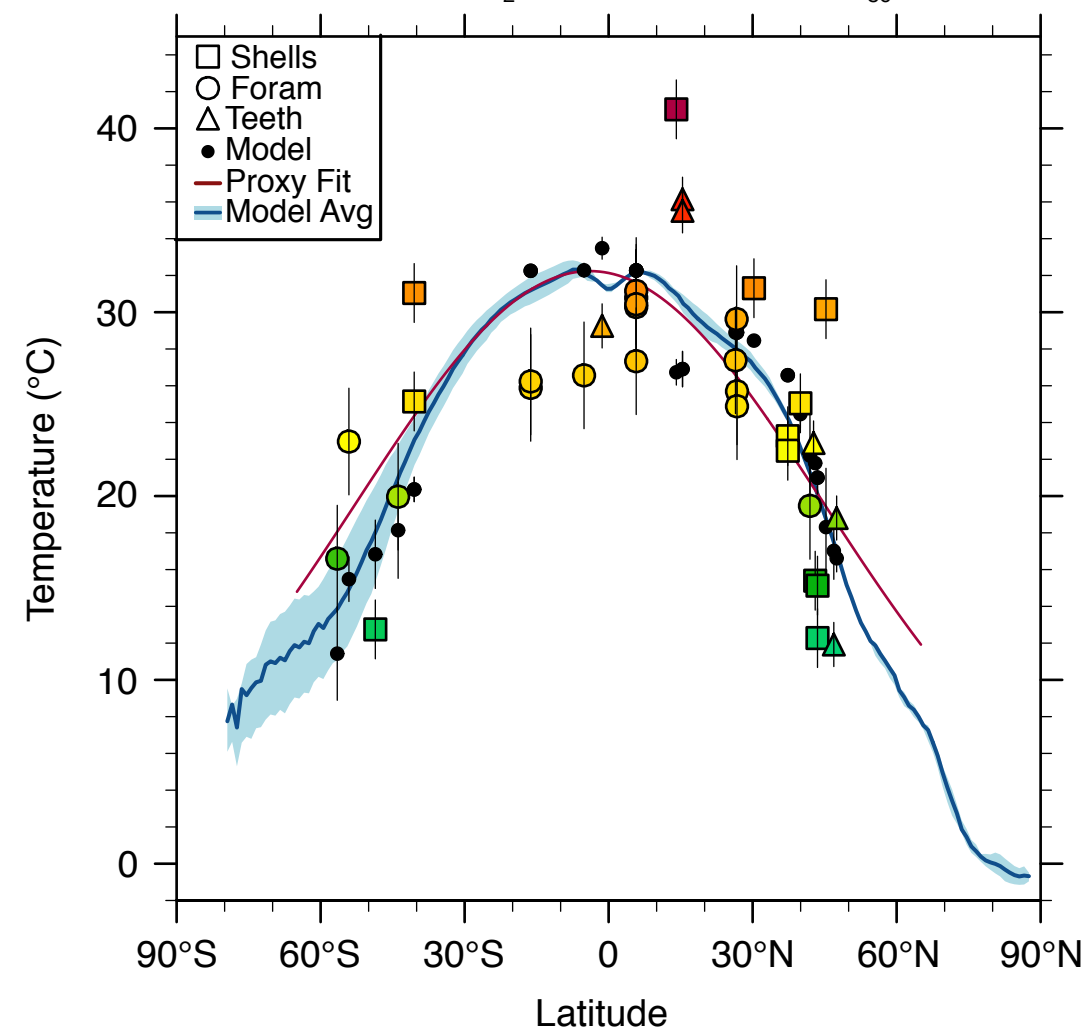


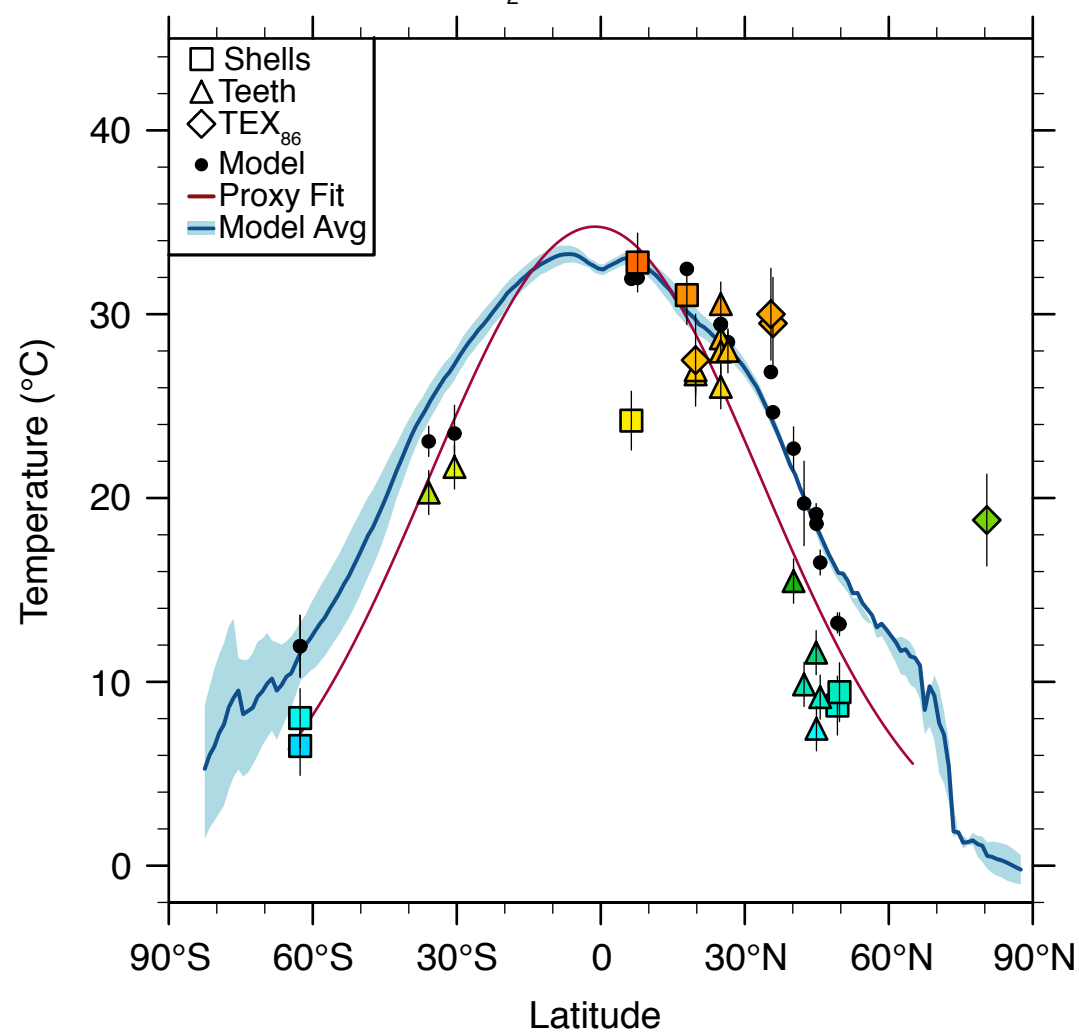
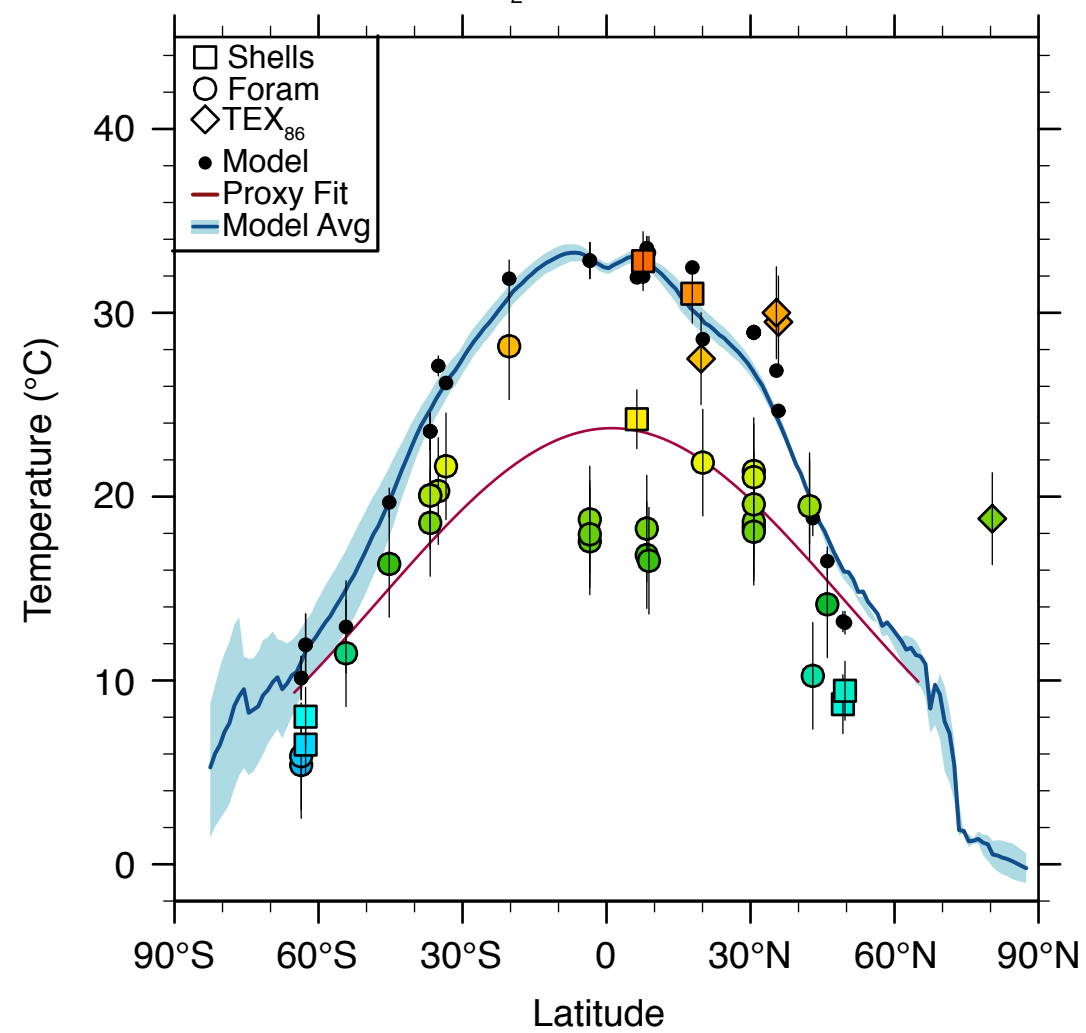
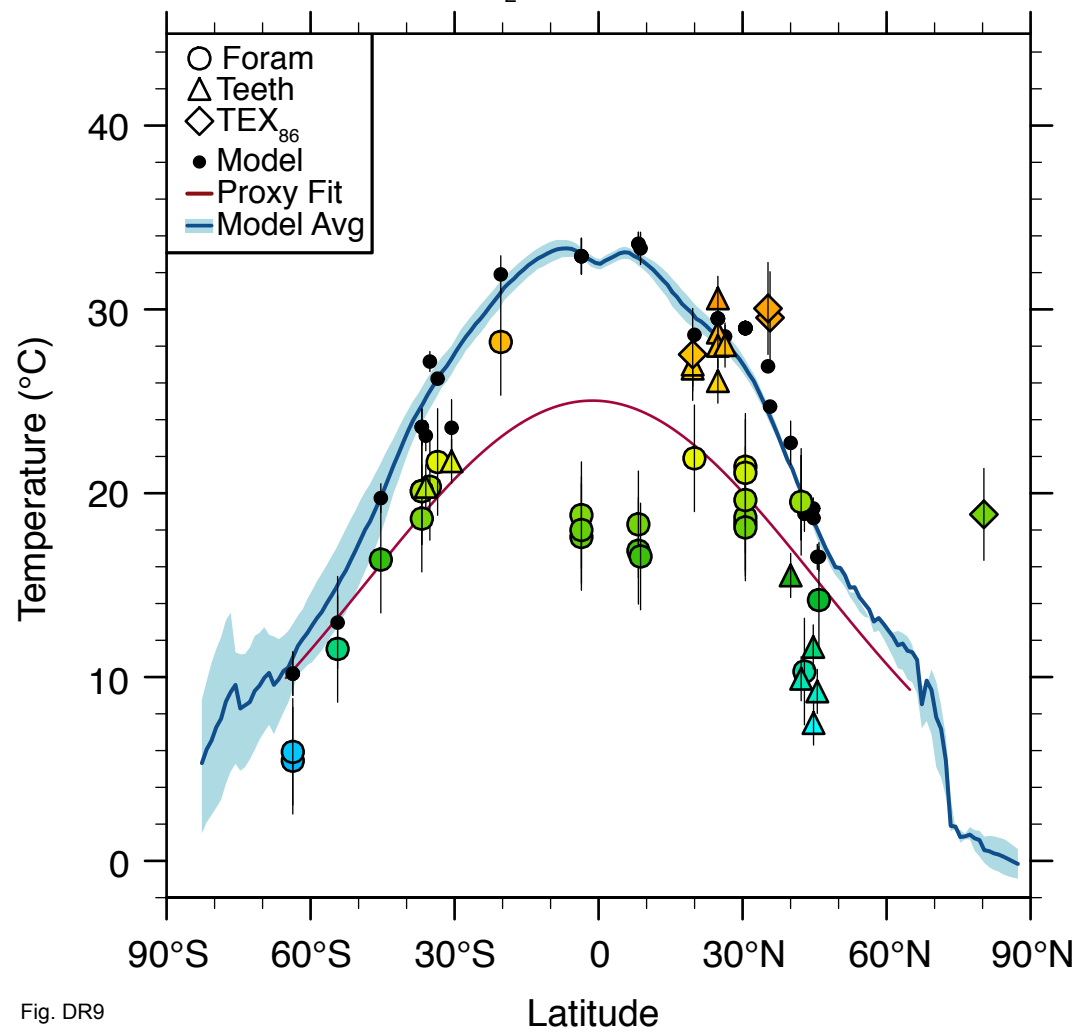
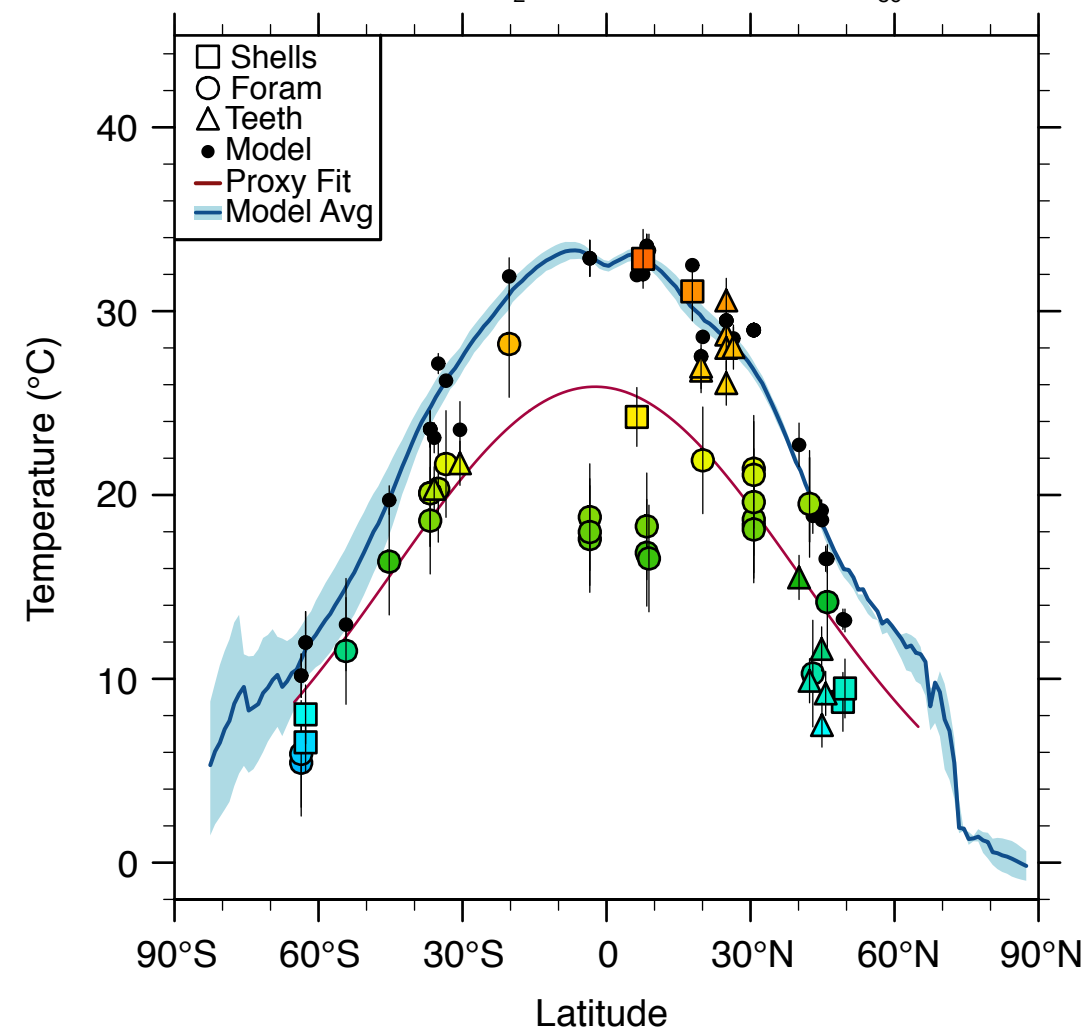
L. MAA2x Ann Avg Sea Ice: HadCM3L SH

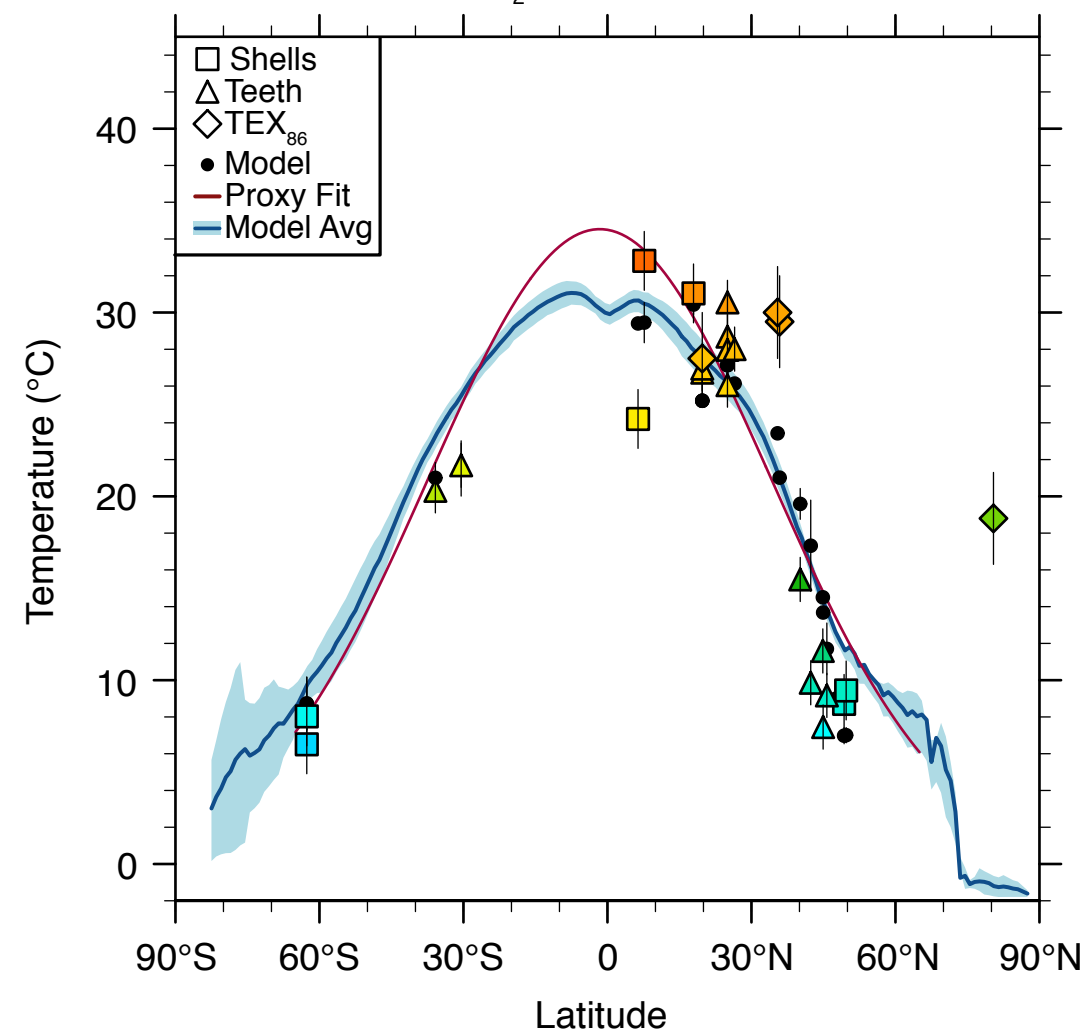
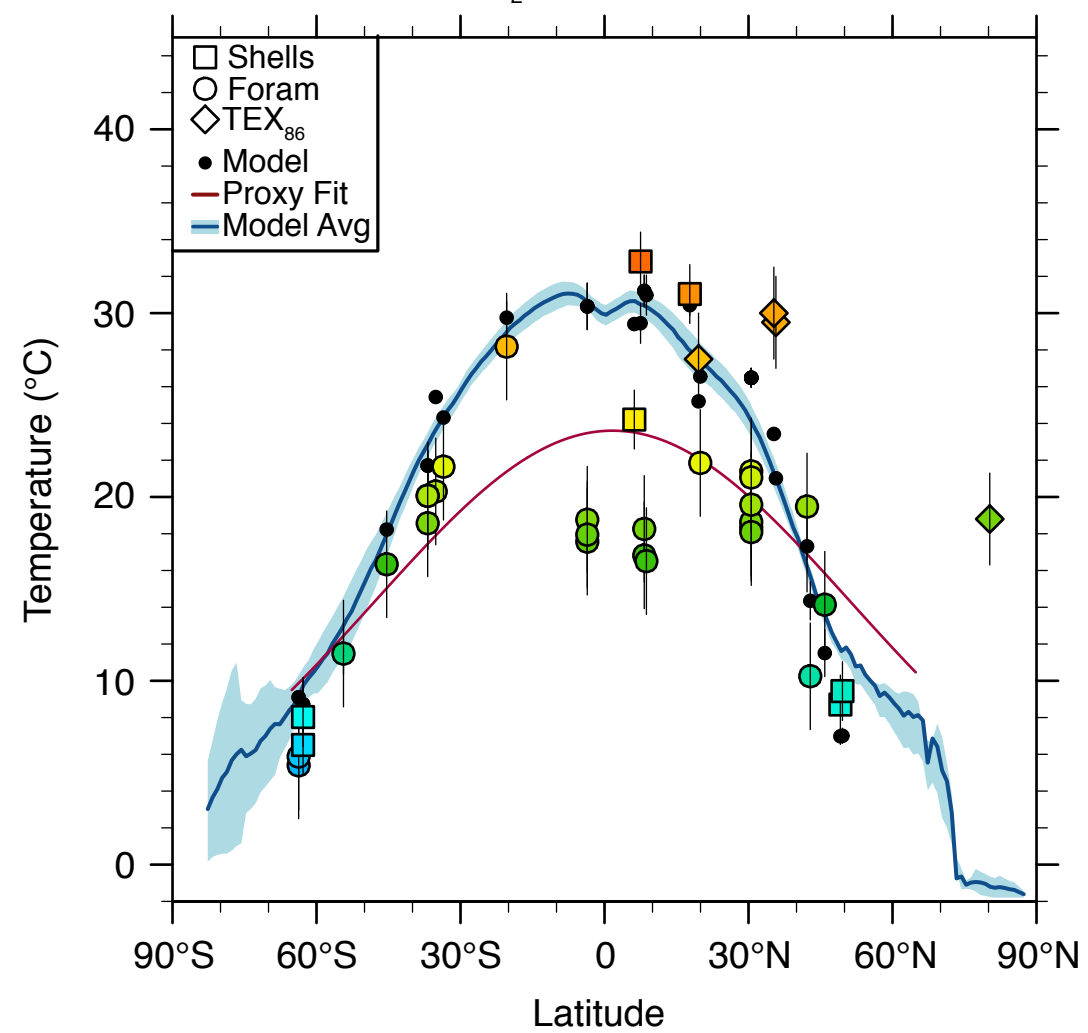
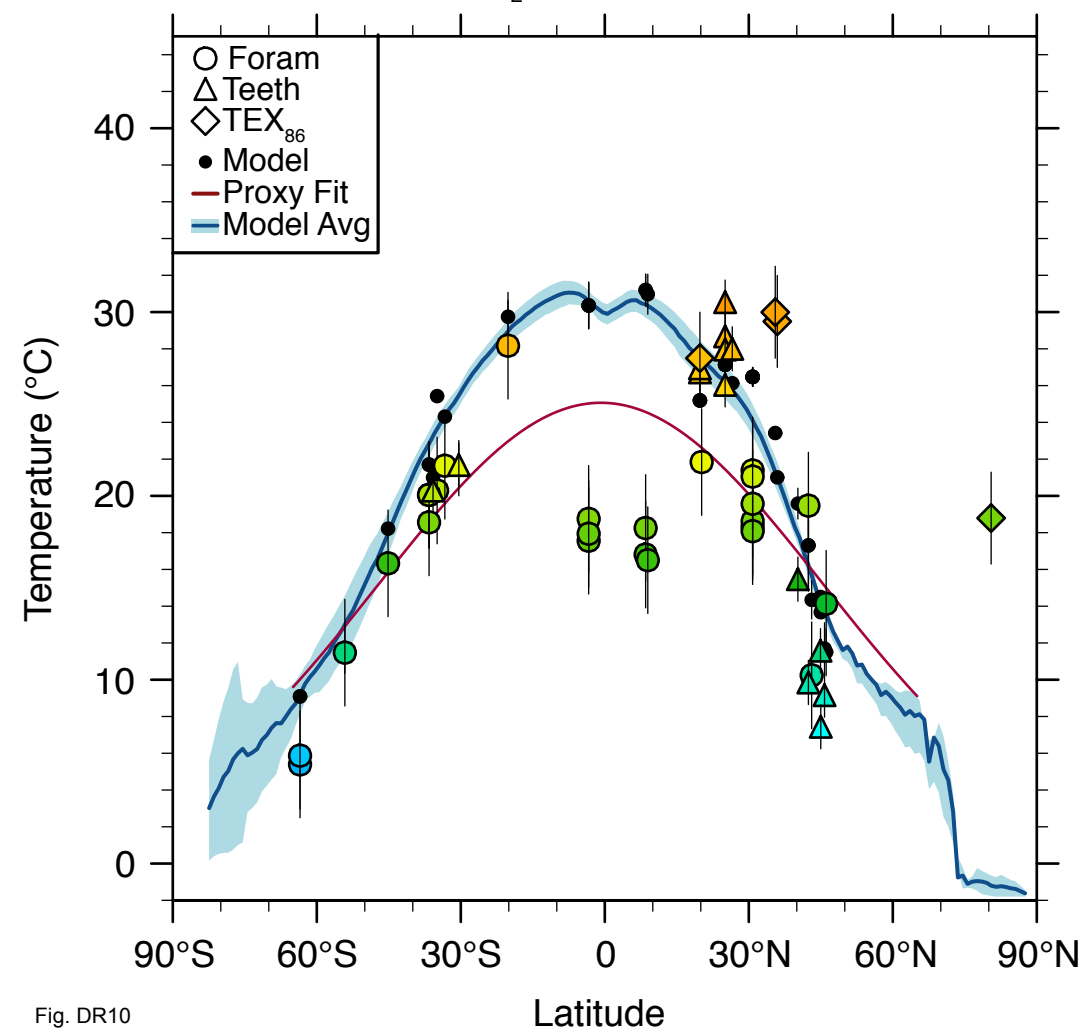
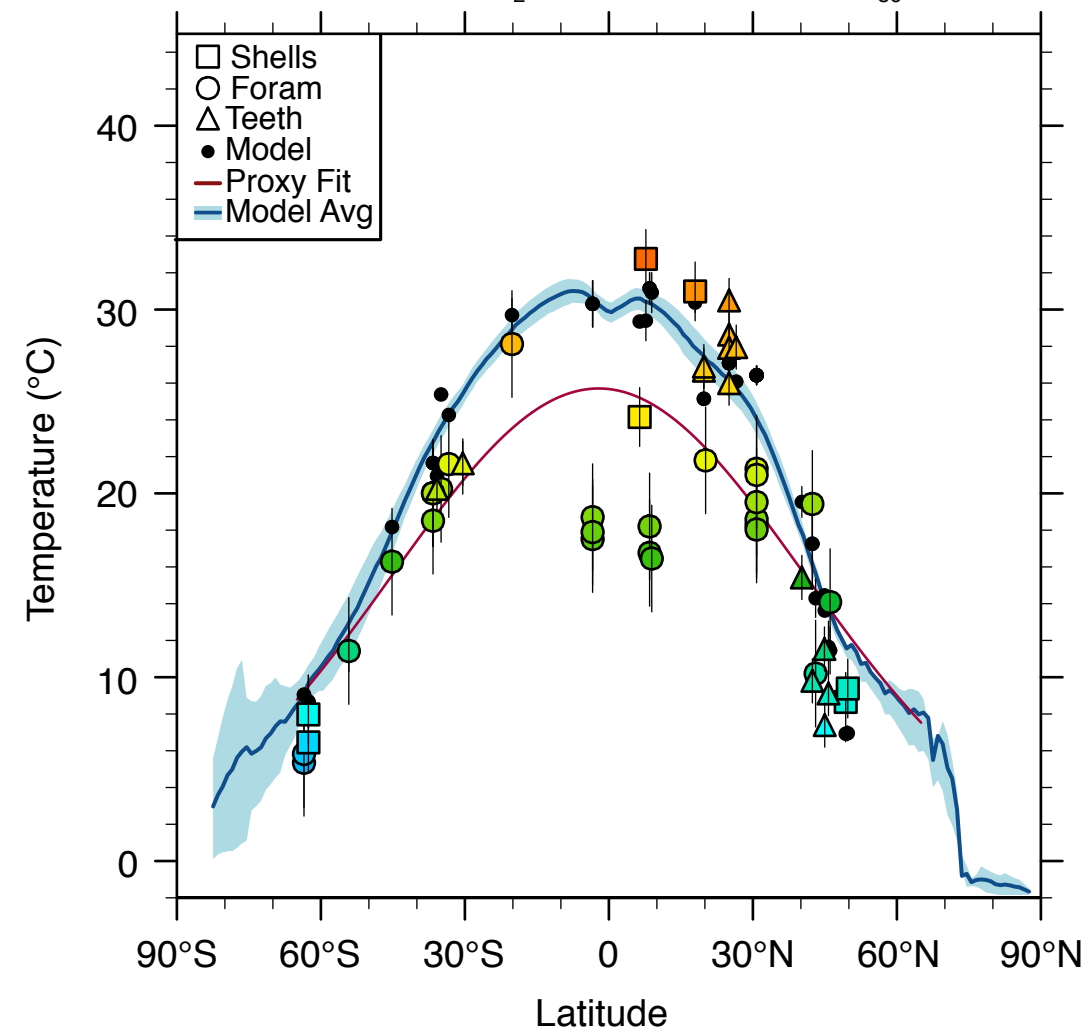


0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9

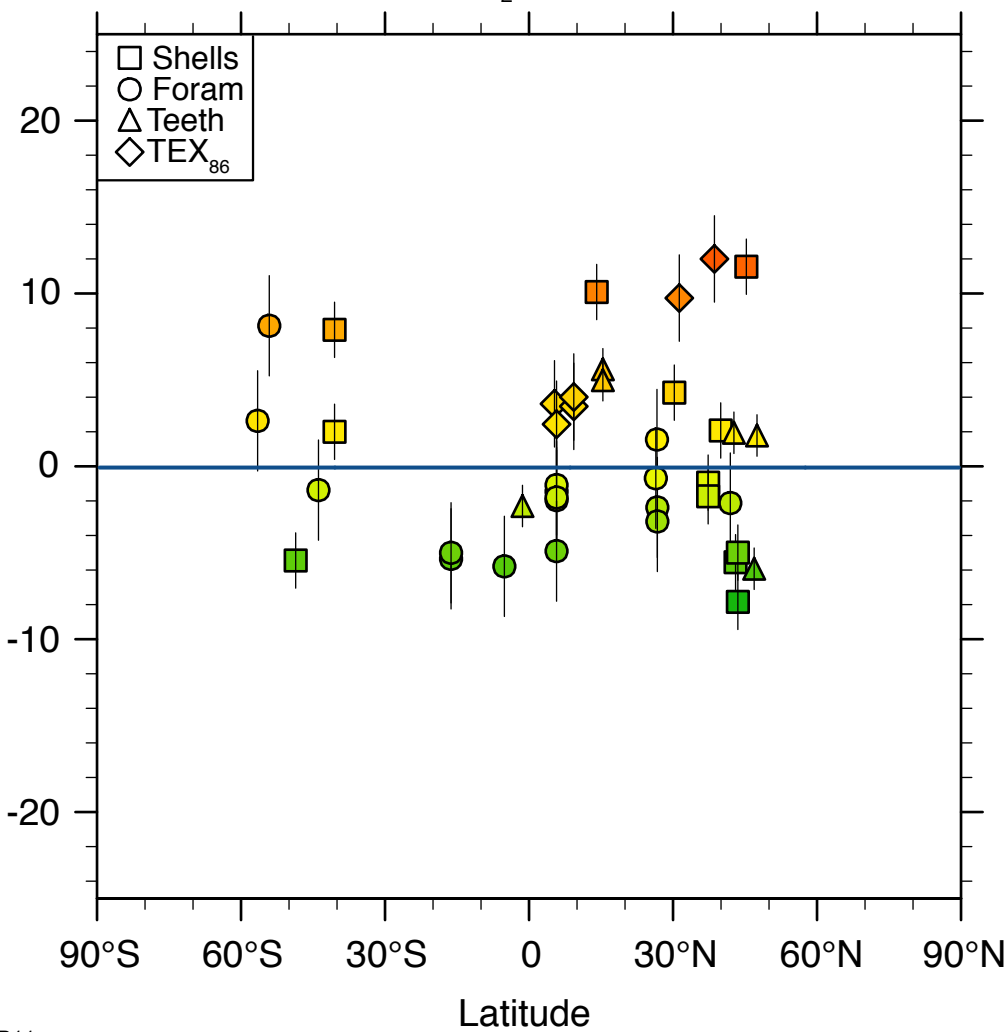
Sea Ice Fraction

A. Cenomanian 4x CO₂ Zonal SSTs: No Forams**B.** Cenomanian 4x CO₂ Zonal SSTs: No Teeth**C.** Cenomanian 4x CO₂ Zonal SSTs: No Shells**D.** Cenomanian 4x CO₂ Zonal SSTs: No TEX₈₆

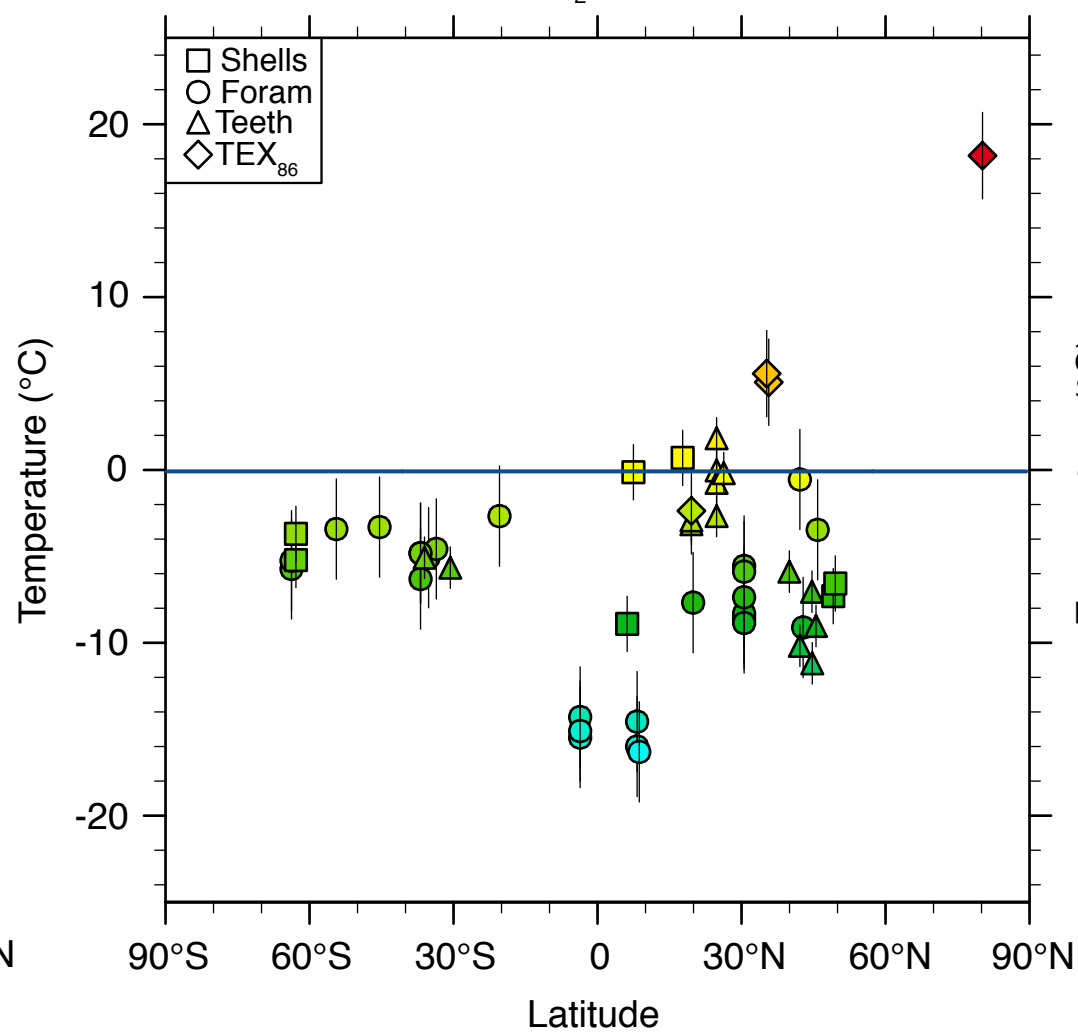
A. Maastrichtian 4x CO₂ Zonal SSTs: No Forams**B.** Maastrichtian 4x CO₂ Zonal SSTs: No Teeth**C.** Maastrichtian 4x CO₂ Zonal SSTs: No Shells**D.** Maastrichtian 4x CO₂ Zonal SSTs: No TEX₈₆

A. Maastrichtian 2x CO₂ Zonal SSTs: No Forams**B.** Maastrichtian 2x CO₂ Zonal SSTs: No Teeth**C.** Maastrichtian 2x CO₂ Zonal SSTs: No Shells**D.** Maastrichtian 2x CO₂ Zonal SSTs: No TEX₈₆

A. Cenomanian 4x CO₂ Zonal SST Differences



B. Maastrichtian 4x CO₂ Zonal SST Differences



C. Maastrichtian 2x CO₂ Zonal SST Differences

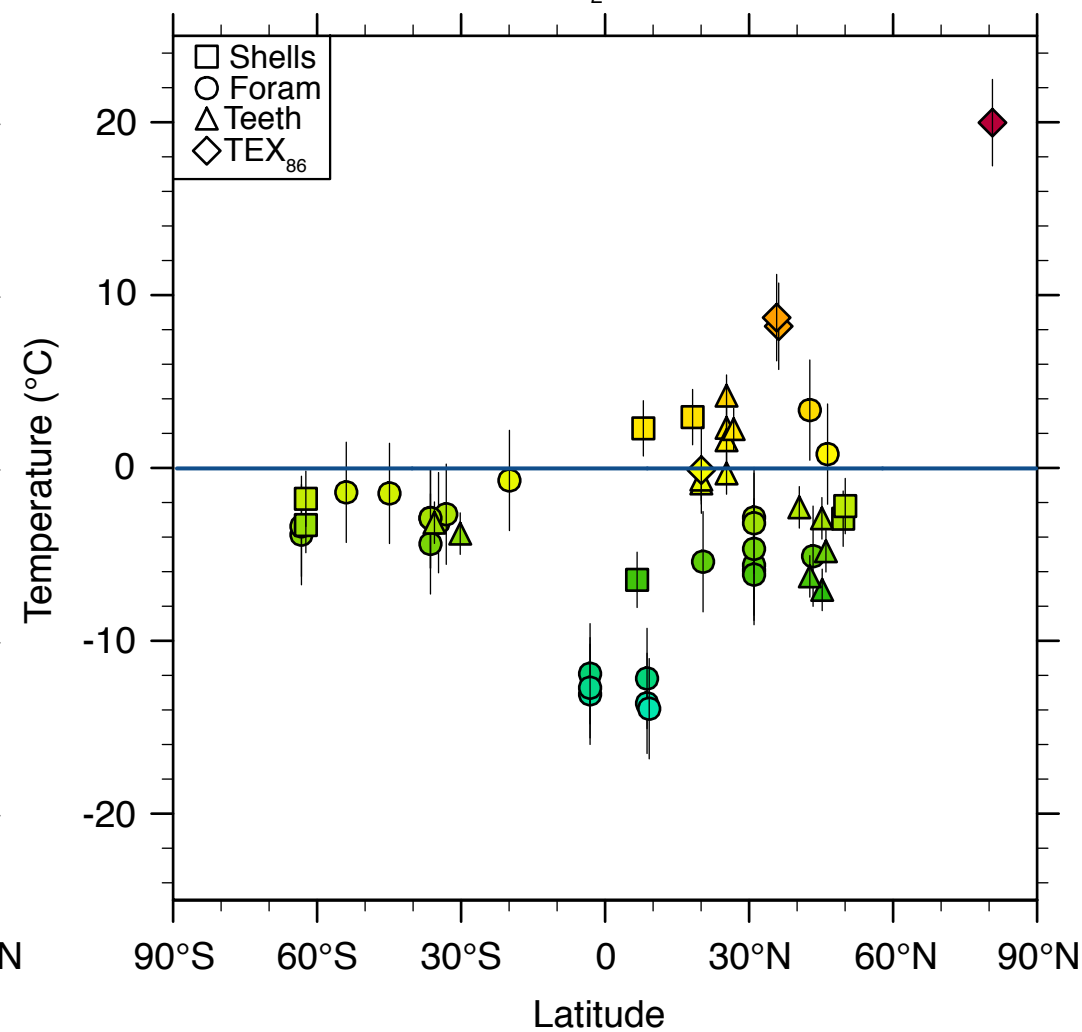


TABLE DR1: MODEL CONFIGURATION AND DATA

Experiment	Age (Ma)	Solar Constant (Wm ⁻²)	CO ₂ (ppmv)	Global MAT (°C)	EQ Temp: 5°S-5°N (°C)	N Pole Temp: 85°-90°N (°C)	S Pole Temp: 85°-90°S (°C)	NH Gradient (°C)	SH Gradient (°C)
Cen4x: CESM	96.4	1353.9	1120	22.80093	30.75579	-10.93816	-4.673659	41.69395	35.429449
Cen4x: HadCM3L	96.4	1353.9	1120	22.17896	31.68976	-12.16977	-7.613354	43.85953	39.303114
Maa4x: CESM	68.2	1357.18	1120	22.92284	31.92628	-9.934456	-5.359563	41.860736	37.285843
Maa4x: HadCM3L	68.2	1357.18	1120	22.33742	32.52404	-8.000755	-7.752418	40.524795	40.276458
Maa2x: CESM	68.2	1357.18	560	19.81563	29.51464	-23.30825	-9.552328	52.82289	39.066968
Maa2x: HadCM3L	68.2	1357.18	560	19.02272	29.29172	-18.09064	-12.0258	47.38236	41.31752

Note: All reported temperatures are mean annual surface temperatures.

TABLE DR2: ALL MAASTRICHTIAN AND CENOMANIAN SST DATA