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An ensemble-based SST nudging method proposed for correcting the subsurface temperature field in climate model

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Abstract
An ensemble-based assimilation method is proposed for correcting the subsurface temperature field when nudging the sea surface temperature (SST) observations into the Max Planck Institute (MPI) climate model, ECHAM5/MPI-OM. This method can project SST directly to subsurface according to model ensemble-based correlations between SST and subsurface temperature. Results from a 50 year (1960–2009) assimilation experiment show the method can improve the subsurface temperature field up to 300 m compared to the quality-controlled subsurface ocean temperature objective analyses (EN4), through reducing the biases of the thermal states, improving the thermocline structure, and reducing the root mean square (RMS) errors. Moreover, as most of the improvements concentrate over the upper 100 m, the ocean heat content in the upper 100 m (OHT_100 m) is further adopted as a property to validate the performance of the ensemble-based correction method. The results show that RMS errors of the global OHT_100 m convergent to one value after several times iteration, indicating this method can represent the relationship between SST and subsurface temperature fields well, and then improve the accuracy of the simulation in the subsurface temperature of the climate model.

Key words: ensemble-based nudging method, ECHAM5/MPI-OM, SST assimilation, simulation of subsurface temperature field

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1 Introduction

Satellite-derived observations, such as SST (sea surface temperature), provide a global coverage of the world ocean with high spatial and temporal resolutions. However, most satellite observations provide only surface information and they may have data gaps. For example, the advanced very high resolution radiometer (AVHRR) pathfinder SST is influenced by cloud. Many approaches have been used to fill these gaps, including data assimilation. A direct method of assimilating SST is to nudge or optimally insert SST into ocean models (e.g., Chen et al., 1997; Rosati et al., 1997; Syu and Neelin, 2000; Tang and Hsieh, 2003; Twigt et al., 2007). This method has some inefficiency, like that it cannot correct the subsurface ocean state or it will lead to serious imbalances between thermal and dynamical fields (Tang et al., 2004).

In order to improve subsurface temperature field through assimilating SST data, different schemes have been proposed. Advanced methods, such as the four-dimensional variational (e.g., Zhu et al., 2002), simplified Kalman filter (e.g., Andreu-Burillo et al., 2007), Kalman filter (e.g., Annan and Hargreaves, 1999), or the ensemble Kalman filter (e.g., Haugen and Evensen, 2002; Zheng et al., 2006; Song et al., 2015), can deliver dynamically consistent profile analysis by using model dynamics as constraints or by calculating the forecast error covariance that is propagated from the previous analysis step based on dynamical models. In doing so, it may be able to produce analyses and forecasts that are much more accurate than some current, simpler data assimilation schemes, which assume that the background error is known a priori and does not vary in time (Zheng and Zhu, 2008). However, there are also some simple schemes being attractive due to the simplicity and computational efficiency of their implementation. The basic idea of these simple schemes is assimilating bogus observations in subsurface that are derived from projecting SST downward (e.g. Ezer and Mellor, 1997; Kelley et al., 2002; Tang et al., 2004; Shu et al., 2009).

Advances in seasonal prediction must come from both model improvements and better constraining initial conditions. The latter is particularly important in the ocean, because the memory for ENSO resides there (Neelin et al., 1998; Zheng and Zhu, 2008). Indeed, the importance of ocean subsurface data in making ENSO predictions has been demonstrated in a number of studies (e.g. Kleeman et al., 1995; Ji and Leetmaa, 1997; Rosati et al., 1997; Zheng et al., 2007; Zheng and Zhu, 2015). The focus of this paper is to explore the use of SST data in constraining the subsurface temperatures with coupled general circulation models

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(CGCMs). Because the relationship between the subsurface temperature field and SST is highly correlated, its inclusion into ocean data assimilation schemes should be promising, and in general its influence has been restricted to the model's SST. Moreover, as SST is available from satellites with a high degree of accuracy, with high spatial and temporal resolution, and in near real time, and they are also relatively cheap in comparison to ocean-based observing systems. Thus, its use in initializing scheme needs to be further studied. The initialization method implemented here is simply to run the coupled model with the SST strongly nudged to observations. Through the proposed ensemble-based nudging scheme, the SST is able to initialize the upper ocean by updating the subsurface temperature field according to its relationship to SST.

2 Model and dataset

2.1 *Model*

In this study, the Max-Planck-Institute (MPI) coupled model ECHAM5/MPI-OM (IPCC version, AR4) is employed. The atmosphere model (ECHAM5) is run at T63 spectral resolution (1.875°×1.875°) with 31 vertical (hybrid) levels. The ocean (MPI-OM) has 1.5° average horizontal grid spacing with 40 unevenly spaced vertical levels. The vertical resolution is based on z-coordinates and it is irregular, with higher resolution (10–100 m) close to the surface that becomes coarser (100–500 m) with depth. Technical details of the ocean model MPI-OM, the embedded sea ice model, and the parameterizations that have been implemented during the transition from the Hamburg Ocean Primitive Equation (HOPE) model (Wolff et al., 1997) to the MPI-OM model can be found in Marsland et al. (2003). Atmosphere and ocean are coupled by means of the Ocean-Atmosphere-Sea Ice-Soil (OASIS) coupler (Valcke et al., 2003). The model does not require flux adjustment to maintain a stable climate, and simulates the mean state, and annual and interannual variability in the Tropical Pacific well. For example, mean deviations from observed sea surface temperature is less than 1K over much of the Tropical Pacific, and the phase and strength of the simulated annual cycle of SST in the equatorial Pacific match observations (Jungclaus et al., 2006). The model has been used in climate predictability and prediction studies (e.g., Keenlyside et al., 2008).

2.2 *Analysis procedures*

A simple nudging analysis scheme has been implemented into the model to generate the initial conditions for the climate simulation and short-term climate prediction. The nudging scheme with the full SST is essentially that described by Keenlyside et al. (2005), the coupled model is run with SST strongly nudged to observations. Between 30°S and 30°N the damping constant equals 0.25 d, poleward of these latitudes the damping constant decreases linearly to zero at 60°S and 60°N (Keenlyside et al., 2005). All model fields, especially for SST strongly related temperatures over the upper oceans, will be adjusted according to the Nudging scheme during the model integrations.

In this work, because the SST nudging scheme cannot directly update the ocean subsurface temperature field, we proposed a new ensemble-based SST nudging scheme for the climate models. This scheme directly projects SST downward to obtain subsurface temperature using correlations based on the ensembles of a 400-year pre-industry climate control simulation (Zheng, 2014) between SST and subsurface temperature. The method was proposed by Ezer and Mellor (1997) who used it to successfully assimilate SST and sea level anomaly (SLA) into the POM (Princeton Ocean Model) in the Gulf Stream region. The surface-subsurface correlation coefficients COR(x, y, z) and correlation factors FT(x, y, z) are defined by

$$\mathrm{COR}=\frac{\overline{(\delta T_{\mathrm{sub}}\delta \mathrm{SST})}}{\sqrt{\overline{(\delta T_{\mathrm{sub}})^2}\,\overline{(\delta \mathrm{SST})^2}}}$$

$$\mathrm{FT}=\mathrm{COR}\times\frac{\overline{\delta T_{\mathrm{sub}}}}{\overline{\delta \mathrm{SST}}}=\frac{\overline{(\delta T_{\mathrm{sub}}\delta \mathrm{SST})}}{\overline{(\delta \mathrm{SST})^2}}$$

where δSST (x, y) and $\delta T_{\mathrm{sub}}(x, y, z)$ are SST and subsurface temperature anomalies at depth z, respectively, which are derived by subtracting the 400-year pre-industry climate control simulation mean. The over bars indicate time average. Figure 1 shows the proxy correlations COR (x, y, z) obtained from the output of pre-industry control simulation. There are good correlations between SST and temperature at the first 3 subsurface layers, with correlation coefficients over 0.9. As depth increases, the correlation coefficients decrease and become less than 0.6 at 80 m depth over a large region (Fig.1). And Fig. 2 shows the correlation factor FT (x, y, z) (i.e., the updating factor to adjust the physical variables according to the variations in SST) at different subsurface layers, and the dominate updates for the subsurface temperatures can only found over the upper 100 m.

During the ensemble-based SST nudging process, the subsurface temperature at each assimilation time is directly calculated from the innovation ΔSST (i.e., the difference between simulated and observed SST at each model step), according to Ezer and Mellor (1997).

$$\begin{cases}\Delta T_{\mathrm{sub}}=\mathrm{FT}\,(x,y,z)\times\Delta\mathrm{SST}\,,\\ T^{\mathrm{a}}_{\mathrm{sub}}\,(x,y,z)=T^{\mathrm{b}}_{\mathrm{sub}}\,(x,y,z)+\Delta T_{\mathrm{sub}}\,,\end{cases}$$

where $T^{\mathrm{a}}_{\mathrm{sub}}(x, y, z)$ and $T^{\mathrm{b}}_{\mathrm{sub}}(x, y, z)$ is the analysis and background temperature at depth z, respectively. ΔT_{sub} is the incremental subsurface temperature directly derived from the innovation ΔSST. In this ensemble-based SST nudging scheme, only the grid points where the first 14 subsurface layers (from 17 m depth to 310 m depth) are used to update the subsurface temperature field. And as shown in Fig. 2, the correlation factor FT(x, y, z) equals to zero when the model depth to 310 m, indicating that no updating will be applied to the physical variables (i.e., subsurface temperate field in this work) at 310 m depth and below.

2.3 *Datasets*

The SST data adopted for both nudging schemes are taken from the Hadley Center Sea Ice and Sea Surface Temperature dataset version 1.1 (HadISST 1.1), which are provided by the Met Office Hadley Centre with 1° horizontal resolution (http://www.metoffice.gov.uk/hadobs/hadisst/). A set of quality-controlled subsurface ocean temperature objective analyses (EN4) (Good et al., 2013) with 1° horizontal resolution is used to compare with the analysis results from 1960 to 2009. Both the SST and EN4 subsurface data are interpolated into the model grids by the bilinear interpolation method.

3 Improvements of the subsurface temperature fields

3.1 *Correlation and RMSE*

In this section, results from the analysis period 1960 to 2009

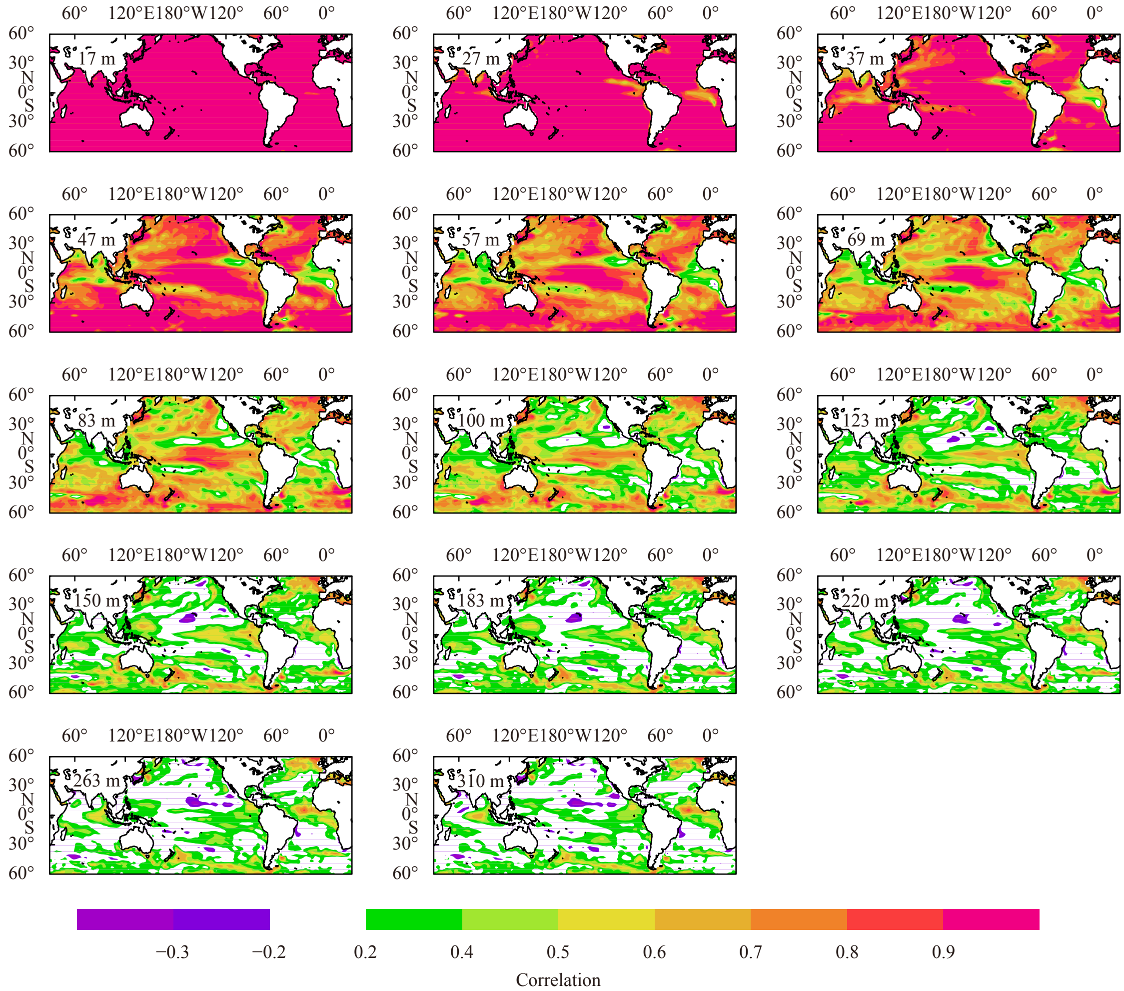

Fig. 1. Correlation (COR in Section 2) of surface-subsurface temperature which derived from the ensembles of a 400-year pre-industry climate control simulation.

are compared with observations. The earlier period is not considered, since sub-surface observations are scarce. The global ocean temperature from surface to 310 m simulated by the analysis were compared with HadISST 1.1 and EN4 temperature objective analyses (Good et al., 2013), and in terms of structure and strength were within the uncertainties of these temperature products.

Improvements in correlation and RMS error between these

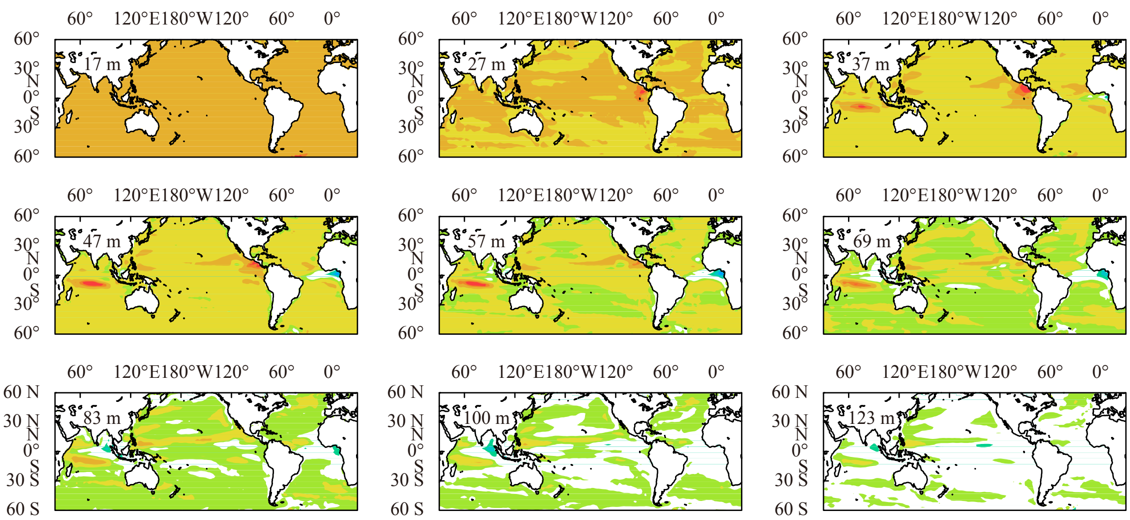

Fig. 2.

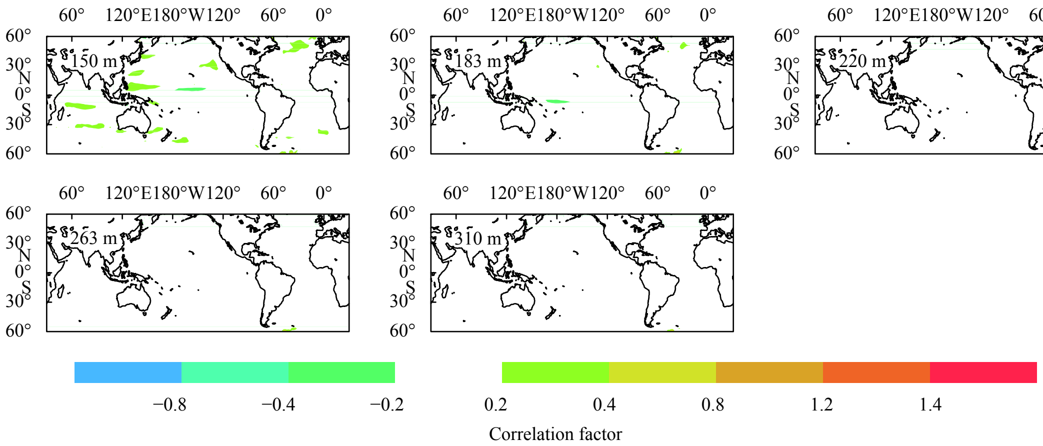

Fig. 2. The correlation factor (FT in Section 2) at different subsurface layers, which is derived from the ensembles of a 400-year pre-industry climate control simulation.

two runs (original SST nudging and new ensemble-based SST nudging) are shown in Figs 3 and 4, respectively. The improvement here means the new ensemble-based SST nudging updating run has a higher simulation skill in correlation and smaller RMS errors than the original SST nudging run. The improvements in correlation can be found within the global mixed-layer, due to the ocean variability is strongly correlated to the variability of SST field. Globally, the improvements are not concentrated at the surface layers, and mostly improved the variability the mixed-layer. Below 100 ms, the significant improvements are mostly concentrated over the Tropical Pacific, and the oceans with deep thermocline structure, such as over the northwest Pa-

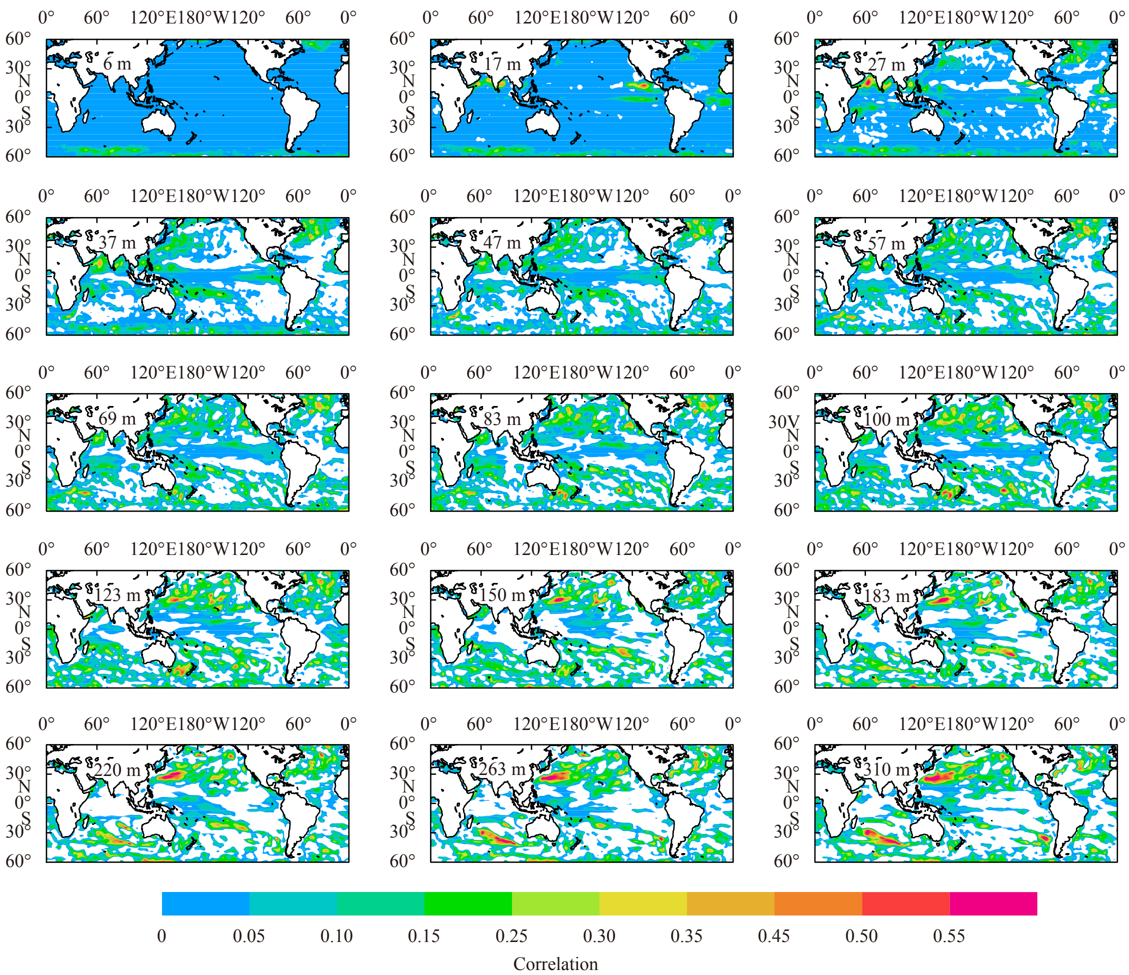

Fig. 3. Improvements in correlation of temperature from surface to subsurface between the new ensemble-nudging scheme and original nudging scheme. The shaded area indicates the simulation skill has been improved in correlation.

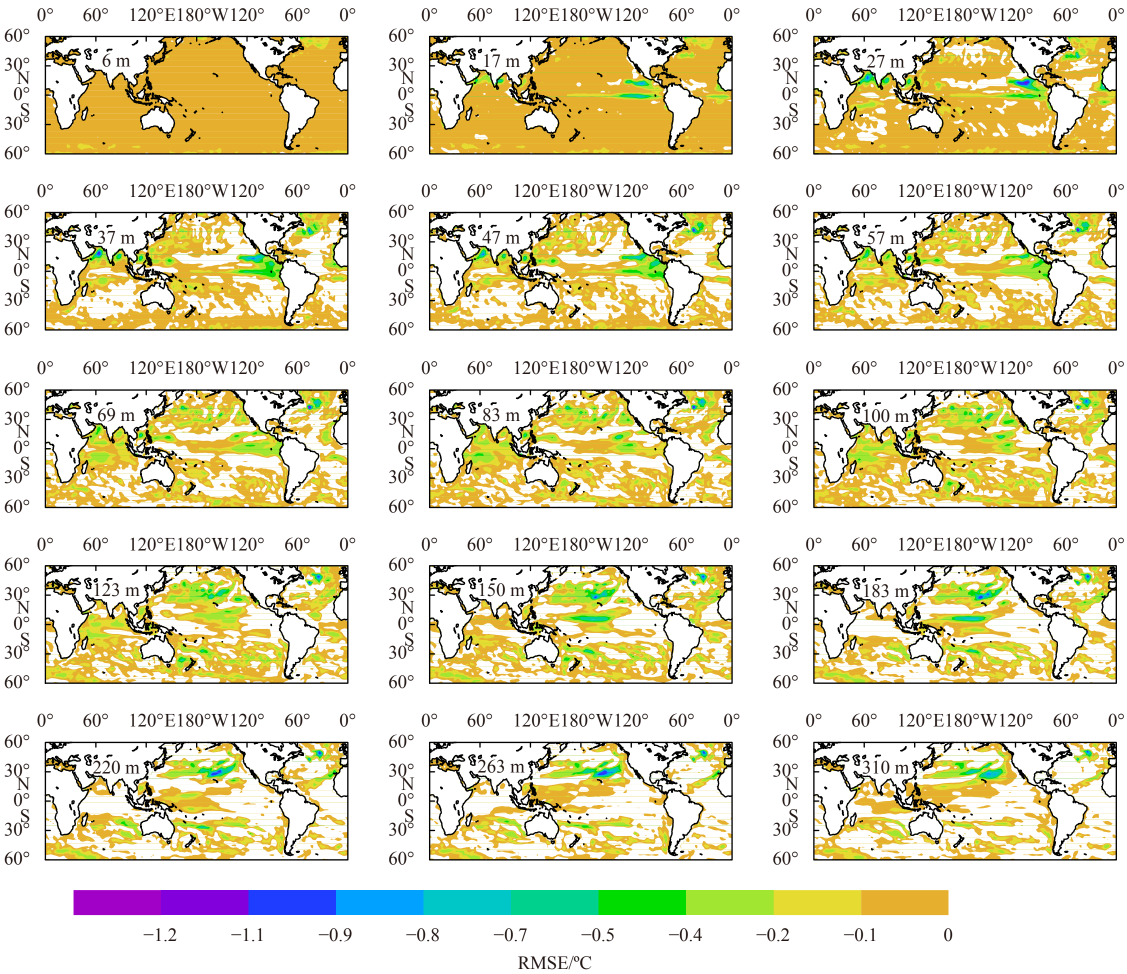

Fig. 4. Reductions in RMSE of temperature from surface to subsurface between the new ensemble-nudging scheme and original nudging scheme. The shaded area indicates the simulation error has been reduced (°C).

cific Ocean, the southern Indian Ocean, and the northern Atlantic Ocean. And the improvements in correlation over these regions can reach to more than 300 ms deep.

Correlations are high improved throughout the equatorial Pacific. In particular, in the Pacific along the thermocline (Fig.5), the improvements of correlation coefficients are ranging from 0.02 to 0.1 (i.e., the percentage of improvement equals to 3%–18%), and the maximum values of the RMS error reduction are around 0.3°C. The weaker correlations about the dateline mark the nodal point in interannual variability in the Pacific. High improved correlations are also found in the subsurface water of the equatorial Indian Ocean and Atlantic Ocean. The reduced RMS errors are relatively weak in the equatorial Indian Ocean and Atlantic Ocean. The difference between the Pacific and the Atlantic are consistent with interannual variability in the Indian and Atlantic on these timescales being significantly weaker. Outside the tropics correlations are weak as expected: In the extra-tropics on seasonal-interannual timescales atmospheric anomalies generally drive SST anomalies.

3.2 *Ocean heat content in upper 100 m*

As most of the improvements concentrate over the upper 100 m, a new diagnostic variable is chosen here (OHT_100 m: average potential temperature in the upper 100 m). To validate whether this ensemble-based subsurface temperture correction method can improve the relationship between surface and subsurface temperature fields, as designed in Table 1, the validation experiments are carried out for improving the OHT_100 m analysis.

For the “Nudg_SST (NSST)” experiment, the observed SST is stored into the modeled SST to generate the analysis fields, as performed as the original SST nudging scheme in Section 3.1. Furthermore, based on the “NSST” experiment, the “Upd_Tsub” experiment can adopt the (1960–2009) long-term simulation results to construct the SST and subsurface temperature relationship, and then we performed the new ensemble-based SST nudging scheme in Section 3.1 to update the temperature fields when restoring the observed SST into the modeled SST. This application also can consider the 20-century condition besides of the pre-industry condition in these experiments. Again, when performing the “Upd_Tsub_1” experiment, we can adopt the long-term “Upd_Tsub” results to construct the SST and subsurface temperature relationship during restoring the observed SST into the model. The “Upd_Tsub_2” and the “Upd_Tsub_3” experiments have the same design as the “Upd_Tsub_1” experiment, and each experiment is adopting the previous experiment to construct the SST and subsurface temperature relationship during the SST nudging process.

Figure 6 compares the variations in RMS errors from different experiments, we can find the RMS errors of these experiments can converge to one possible value, and the SST nudging scheme

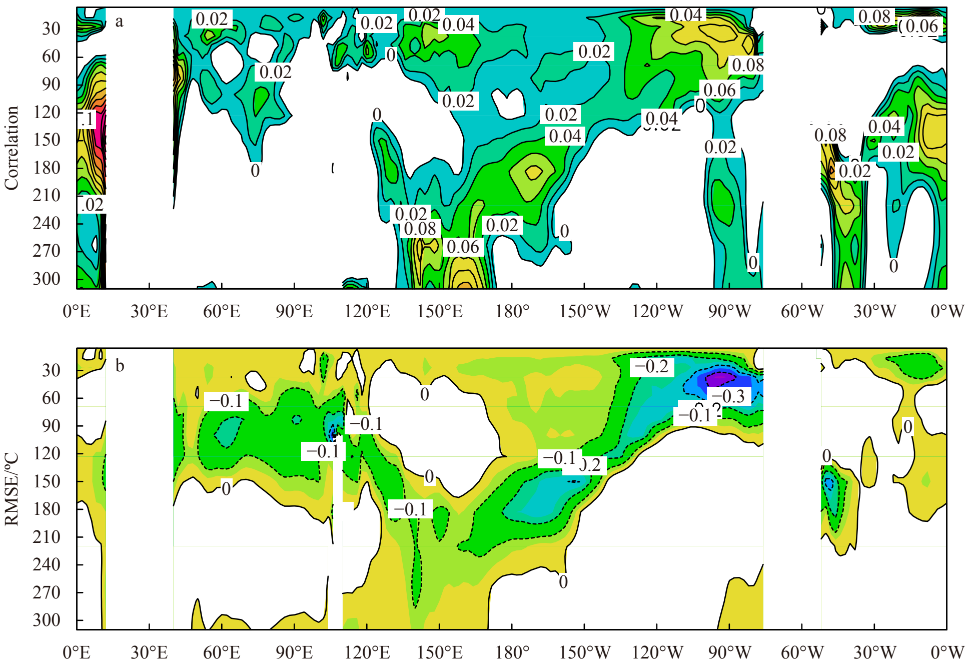

Fig. 5. Simulation differences over the tropical oceans between the new ensemble-nudging scheme and original nudging scheme, (a) is for the improvements in correlation coefficients of temperature, and (b) is for the reductions in RMS errors. The shaded area in (a) indicates the simulation skill has been improved in correlation, and the shaded area in (b) indicates the simulation error has been reduced over the tropical oceans (°C).

Table 1. Experiment design for the five analysis experiments

Experiment Name	Experiment description
Nudg_SST (NSST)	Restoring the observed SST into the modeled SST to generate the analysis fields
Upd_Tsub	Adopting the long-term NSST results to construct the SST and subsurface temperature relationship, and updating the temperature fields when restoring the observed SST into the modeled SST
Upd_Tsub_1	Same as in the Upd_Tsub experiment, but adopting the long-term Upd_Tsub results to construct the SST and subsurface temperature relationship
Upd_Tsub_2	Same as in the Upd_Tsub experiment, but adopting the long-term Upd_Tsub_1 results to construct the SST and subsurface temperature relationship
Upd_Tsub_3	Same as in the Upd_Tsub experiment, but adopting the long-term Upd_Tsub_2 results to construct the SST and subsurface temperature relationship

gets the worst score of all the experiment. There are nearly no differences in RMS errors between the Upd_Tsub_2 and Upd_Tsub_3 experiments, indicating that the OHT_100 m has been updated to a limit due to the directly adjusting of the subsurface temperature field. Also, as shown in Table 2, the temporal averaged RMS error for the OHC_100 m over global, or over 60°S–60°N, or over 30°S–30°N, can all access to a minimal value, and the differences in the temporal averaged RMS error of OHC_100 m between the Upd_Tsub_2 and Upd_Tsub_3 experiments can be neglected. These comparisons indicate this ensemble-based SST nudging method can represent the relationship between SST and subsurface temperature field well, and can update the temperature field over the upper ocean to an optimal state for initialization.

4 Discussion and conclusions

In this work, we have compared a general SST nudging scheme with a new proposed ensemble-based SST nudging scheme for the climate model's initialization using the ECHAM5-MPIOM model. Owing to the strongly mixed over the upper oceans globally, the correlation between SST and subsurface temperature is good over the upper 100 m, and also useful for several deeper mixed-layer regions (Northwest Pacific, Southern Indian, and Northern Atlantic oceans). Thus, projecting SST directly downward to subsurface in the ensemble-based SST nudging scheme can help to update the subsurface temperature field directly when restoring the SST observation into the climate model, and which is a more effective way compared to the original SST nudging approach, showing that the new scheme can correct temperature in the mixed layer to some extent. Compared to the original SST nudging scheme, the new scheme is better at achieving the RMS error reduction because more innovation is obtained in the mixed layer, which makes the surface increment decay more slowly in time. And at surface level, the new scheme can improve the distribution of SST by correcting the cold bias in the control run and reducing the RMSEs by about 50% (not shown). Moreover, since the statistical relationship between surface and subsurface decays with depth, the updating of the subsurface temperature is most concentrating over the upper 100 m. However, considering that baroclinic modes always exist in real ocean, the projection of out-of-phase relationship in the scheme is smoothed. The following work of this paper is to explore the use of SST data in initializing seasonal forecasts with coupled general circulation models (CGCMs), and since the proposed simple initialization method is promising, the realistic seasonal

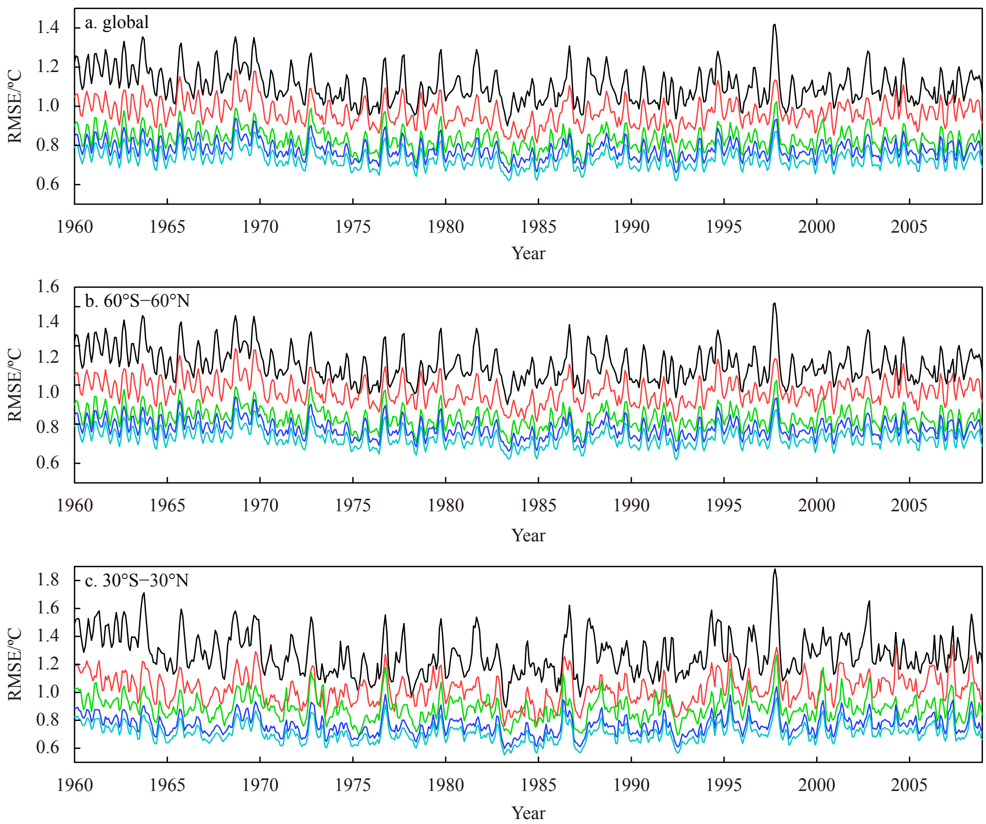

Fig. 6. Temporal variations in the averaged RMS error of the OHC_100 m over global, or over 60°S–60°N, or over 30°S–30°N from five different analysis experiments. The black line represents the results from the NSST experiment, the red line represents the results from the Upd_Tsub experiment, the green line represents the results from the Upd_Tsub_1 experiment, the blue line represents the results from the Upd_Tsub_2 experiment, and the light blue line represents the results from the Upd_Tsub_3 experiment, respectively.

Table 2. Temporal averaged RMS error of the OHC_100 m for each experiment

Experiments	Temporal averaged RMS error for the OHC_100 m/°C		
	Global	60°S–60°N	30°S–30°N
Nudg_SST (NSST)	1.09	1.07	0.98
Upd_Tsub	0.96	0.94	0.84
Upd_Tsub_1	0.83	0.82	0.77
Upd_Tsub_2	0.78	0.76	0.72
Upd_Tsub_3	0.75	0.74	0.69

predictions by adopting this initialization scheme should be carried out in future works.

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