Improving High-Latitude Sea Surface Height Data Assimilation: Part I Selective Synthetics

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ABSTRACT: Modeling systems with data assimilation are often used to estimate the ocean state. When assimilating sea surface height, these systems include assumptions about subsurface ocean structure that are valid at low- and mid-latitudes, but may falter due to unstratified subsurface conditions at high latitudes. The systems are also dependent on the validity (number and quality) of historical data, which provide climatological covariances linking sea surface height and variability in subsurface ocean structures through a one-dimensional variational estimation system. This analysis uses an Observing System Simulation Experiment (OSSE) framework to examine how sea surface height observations at high latitudes are currently being used. First, are the historical restrictions on what data can be used and what must be discarded valid? What would be gained, if we were able to accurately extract profile information from discarded data and assimilate them? Additionally, one needs to consider the effects of the Arctic-amplified warming that may be making current climatologies and covariances obsolete. Overall, the study will help exploit Arctic measurements to the maximum extent possible to create an integrated estimate of the Arctic system.

1. Introduction

Obtaining an accurate estimate of the ocean state is the goal of data assimilation in operational ocean forecasting systems. As data are sparse and difficult to obtain, an accurate data assimilative analysis system begins with our understanding of the physical basis of ocean dynamics, and then integrates an analysis of observations from many sources, including satellite and in situ data. System development proceeds from many directions: increasing resolution, improving physical representations or parameterizations, expanding datasets, and adapting assimilation processes to include new and more varied types of data. It is sometimes necessary to reconsider past assumptions and ensure that they are still reflective of the evolved assimilative system, the associated historical dataset, and the environment in which it is being used. Here we will consider assimilation of sea surface height at higher latitudes. In the assimilation system considered in this manuscript, sea surface height is converted into synthetic temperature (T) and salinity (S) profiles, which are then assimilated into the model (Helber et al. 2013; Metzger 2014). Some assumptions that are valid and accurate for middle and lower latitudes, such as the dominance of temperature in determining stratification, may not accurately represent the higher-latitude oceanic structure. Similarly, through polar amplification of global warming, the oceanic structure at higher latitudes is changing at a faster rate than is the case at lower latitudes (Rantanan et al. 2022). This is particularly relevant when one considers the reliance of models and assimilation methods on climatology to set the background ocean state. If a climatology is outdated due to global change, using it to estimate the current ocean state will introduce a systematic bias.

This manuscript is Part I of two paper that examine the impact at high latitudes of some of the underlying assumptions built into the Global Ocean Forecasting System (GOFS), the United States Navy's operational system for assessing the current ocean state (Metzger et al. 2017). Specifically, two issues are examined. First, does the relatively simple metric employed to estimate stratification result in discarding data that could provide useful information on ocean structure? Second, does the climatology being used by the system introduce a bias into results, due to changes in high latitude Arctic structure resulting from climate change? These issues will be addressed using an Observation System Simulation Experiment, or OSSE, framework. The details of this framework will be examined in Section 2. Section 3 will discuss synthetic profiles as they are used in the forecasting system. Section 4 will look at details of the results of these experiments to identify spatial patterns and how these might relate to regional differences. Section 5 will include discussion and conclusions. Part II addresses the impact of replacing data-based vertical covariances with model-based ones.

2. OSSE Framework

An Observation System Simulation Experiment, or OSSE, is a framework for examining the performance of an assimilative observational system. In such a system, the first step is to run a non-assimilative model for a number of years. The resulting model output is known as the Nature Run, and it constitutes the known "correct answer" for testing the system. The Nature Run is then sampled in a way that mimics the observational system in question. These "simulated observations" are assimilated by the system being tested. In the real world, it is hard to fully assess the efficacy of an assimilative model because of a lack of knowledge of the "right answer"; in the OSSE framework, the Nature Run provides a complete ocean state to which the assimilating output can be compared for verification. The results of the assimilation of the simulated observations can be compared back to the Nature Run, allowing a full assessment of model performance. By varying which "observations" are included, one can determine the individual influence of different times, locations, and types of data, which can be used to make decisions as to which data are of most use in understanding specific regions or phenomena.

In this case, we choose to analyze the details of our assimilation of SSH data at high latitudes (above 40°N) in the Northern Hemisphere. The region is shown in Fig. 1. The bulk of observations in this region come from satellite altimetry over the ocean, as well as satellite-derived ice concentration in the ice-covered or marginal ice zones. Satellite sea surface temperature (SST) is also available, though dependent on cloud cover. In situ observations in these regions are few and far between, and strongly seasonally dependent. As will be shown, while satellites give good coverage of the region, much of the sea surface height data is currently being discarded due to a restriction built into the assimilative code. This restriction will be examined.

The Nature Run used for this project is described in detail in Fine et al. (2023). To summarize, it is a global ocean/sea-ice model that uses the Parallel Ocean Program 2 (POP2) model and the Los Alamos sea ice model 5 (CICE5) as component models coupled together in the Department of Energy (DOE)'s Energy Exascale Earth System Model "HiLAT" framework (E3SMv0-HiLAT;

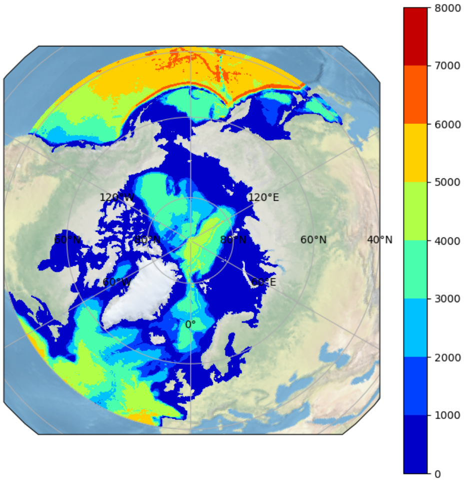

FIG. 1. Bathymetry of the Arctic Cap region where the OSSE model was run.

Hecht et al. (2019)) . The model's horizontal grid is configured to have nominal resolution close to 8 km at the equator reducing to 2 km at the poles. The model is designated as the "ultrahigh 8to2" or UH8to2. It was initialized in August 2016. The initial condition was from the Navy's GOFS3.5 system (Metzger et al. 2020), and the atmospheric forcing is from JRA55-do (Tsujino et al. 2018).

The OSSE model is based on the Hybrid Coordinate Ocean Model (HYCOM, (Bleck 2002; Chassignet et al. 2003)), also coupled with CICEv5 (Hunke et al. 2015). It has a nominal resolution of 1/12° at the equator, which is roughly 2 km at the poles. The region used here is known as the Arctic Cap, including all latitudes north of 40°N. Each OSSE was run for one year, starting on January 1, 2017. The setup of this model is intended to mirror the Navy's operational system, so that it can be used to evaluate that system's accuracy. Therefore, initial and boundary conditions are supplied by GOFS, which (as stated above) is the Navy's operational system for ocean state (Chassignet et al. 2009; Metzger 2014), and the atmospheric forcing is from the Navy Global Environmental Model (NAVGEM).

3. Synthetic profiles

In the Navy's assimilation system (Navy Coupled Ocean Data Assimilation, or NCODA), sea surface height information is not assimilated directly (Cummings 2005). Instead, a system called

Improved Synthetic Ocean Profiles (ISOP) (Helber et al. 2013) is used. This system creates synthetic profiles from altimetric sea surface height anomalies. The synthetic profiles are derived from inputs of sea surface temperature (SST) and sea surface height anomaly (SSHA) using a one-dimensional variational analysis based on vertical covariances empirically derived from historical in situ observations. The results are synthetic profiles that are an anomaly from climatology at the location and month of the input SST and SSHA data. In essence, the synthetic profiles are an answer to the question: in this location, what subsurface ocean structure is most likely to provide the observed sea surface height anomaly? As an example, consider a midlatitude location where the sea surface height is anomalously high. This is likely to indicate the passage of a warm-core mesoscale eddy, depressing the thermocline and increasing subsurface height. The synthetic profiles of temperature and salinity would reflect the most likely values, given the magnitude of the anomaly. The synthetic profiles created in this way are then assimilated.

While the system generally works well, there are some shortcomings. First of all, the construction of the covariances on which ISOP is based requires ocean observations, which are sparse in the high latitudes. Second, the construction of synthetic profiles is also based on climatology; if the sea surface height is not anomalous, the profile assimilated will closely resemble the climatological mean for that location. Given the extent and magnitude of Arctic warming, it is reasonable to question whether the current state of the ocean is well-represented in climatology that may be partially based on historical data, taken when the state of the Arctic was fundamentally different than it is now. Consequently, one of the focuses of the experiments performed here was to determine how well ISOP is functioning, and what steps could be taken to change the covariances or climatologies associated with the system.

Another aspect of ISOP that will be examined is an assumption originally developed for the prior Modular Ocean Data Assimilation System (MODAS) (Fox et al. 2002). MODAS developed the process by which synthetic profiles are determined from climatological correlations of SSHA and SST with subsurface T and S structure, derived also from historical in situ observations. The construction of synthetic profiles, for both ISOP and MODAS methods, assumes that changes in altimetric height are steric changes in a stratified ocean. In the mid- and low-latitudes, these assumptions are valid, as was borne out over years of use and validation of both methods (Fox et al. 2002; Helber et al. 2013). In the unstratified high latitude ocean, the MODAS method was not as

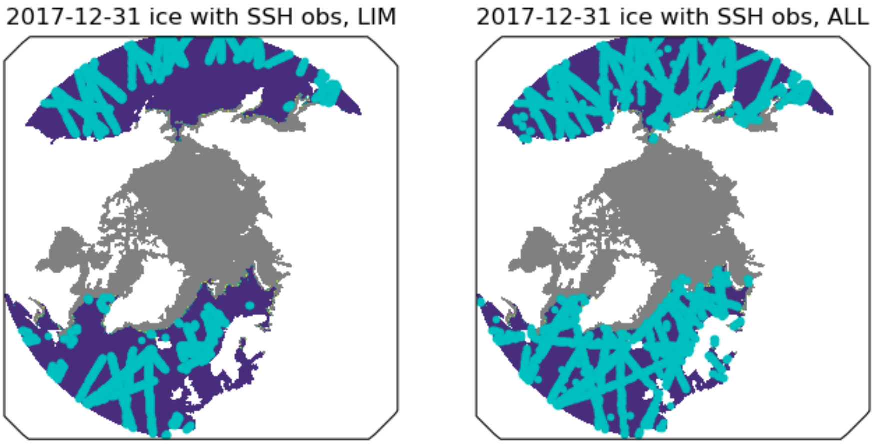

FIG. 2. Left: locations where synthetic profiles were assimilated after the Tcheck for stratification was applied on Dec 31, 2017. Right: all profiles available on Dec 31, 2017.

reliable; consequently, a simple check was introduced into the assimilation process that is still used in ISOP: if a synthetic profile is found to have a temperature difference between surface and 1000 m of less than 3°C (i.e. weak stratification), the profile is discarded and nothing is assimilated. We will refer to this metric of surface temperature minus temperature at 1000 m hereafter as the Tcheck. At high latitudes, where temperatures are generally very cold and do not vary a lot with depth, this means a significant portion of data is being discarded (Fig. 2). The ISOP methods, however, have a better chance of capturing the SSHA response at high latitude than MODAS, through the 1D variational approach that requires the synthetics to have a steric height to match the input SSHA (see Part II of this paper for details). The success of this approach is still, however, strongly dependent on the historical in situ observational data availability at high latitudes and may still have issues in some parts of the ocean.

At high latitudes, the Tcheck may well be less than three degrees, but that does not necessarily mean a lack of stratification. There are complex dynamics in play, including freshwater discharge from melting sea ice and water mass dynamics. The water is quite cold, and stratification is often controlled by salinity rather than temperature; even when surface temperature and temperature at depth are similar, there is sometimes large subsurface variability that can be observed, understood, and incorporated into synthetic profiles. On the other hand, at some locations, such as deep water formation locations in the Labrador Sea, the water column truly is unstratified, and attempting to create synthetic profiles will produce less-than-accurate results. Therefore, determining where and when to use synthetic profiles is a complicated question. The use of the three-degree metric is a shorthand that does ensure that ISOP is not applied in places where it would not be applicable, but it also limits the use of ISOP in places where it could be valid and useful.

In light of these questions about synthetic profiles and their use, four OSSEs were designed to examine the way we use the data already available to us. In the first case, at all locations where SSH is available and the observations have Tcheck greater than 3°C, temperature and salinity profiles directly from the nature run are assimilated (TEMP LIMITED). This eliminates the use of ISOP, and examines how well we could replicate the Nature Run if ISOP were, in essence, perfect. In the second case, ISOP is applied the same way it is currently applied operationally, by creating synthetics from inputs of SST and SSHA sampled from the Nature run and including the 3-degree threshold (ISOP LIMITED). Tcheck is used to eliminate locations where the synthetic profile is deemed unstratified. In the third case, temperature and salinity from the nature run are assimilated directly as in the first case, but Tcheck is removed, such that profiles are assimilated at all SSH locations, regardless of the temperature profile (TEMP ALL). And in the final case, ISOP is used, but without Tcheck, such ISOP is now being applied, by creating synthetic from surface SST and SSHA, in cases where profiles would have been discarded (ISOP ALL). By examining the differences between these four cases and the nature run, we can determine the utility of ISOP at high latitudes, assess the impact of Tcheck, and gain an overall better understanding of how effective our use of high latitude data is.

4. Experimental results

a. Overall spatial patterns

As a first step, we evaluate the average root-mean-square (RMS) difference between each of the four OSSEs and the truth, i.e. the Nature Run, at each gridpoint over the Arctic for one month (December 2017). To obtain these maps (Figure 3), the OSSE outputs were interpolated spatially (vertically and horizontally) onto the Nature Run POP grid. The maps shown in Figure 3 are RMS differences at a depth of 130 m. As will be emphasized in later sections, this depth was chosen because it is near the location of the thermocline, so larger differences may be expected. The RMS maps can then be differentiated from each other. First, we consider the map of TEMP ALL minus TEMP LIMITED. On this map (Figure 3a), a negative number (blue) indicates the TEMP LIMITED RMS difference from the Nature Run is higher than that of the TEMP ALL; that is, the TEMP ALL is a more accurate result. As one might expect, the map is mostly blue. If one was able to assimilate accurate profiles in more places, overall results would be more accurate.

The second map to consider is a comparison between ISOP ALL and ISOP LIMITED (Figure 3b). This metric of ISOP ALL RMS minus ISOP LIMITED RMS will be referred to as RDIFF for the remainder of the manuscript. This gets to the heart of the question: are there locations where by applying ISOP, regardless of the Tcheck, we could more accurately depict the ocean state? The answer is not entirely clear. In many locations the values are low and there is a mix of red and blue, but there are some locations where consistently large high or low values invite further investigation. Looking first at the Labrador Sea, it is evident that ISOP does improve the T and S structures in the center of the Labrador Sea, but that it degrades the results nearer to the coastline. Similarly, there is a region of blue (indicating improvement) in the Okhotsk Sea on the Pacific side of the map. On the other hand, bright red on the eastern side of the Kamchatka peninsula indicates that using full ISOP makes the results worse.

The regions of the ocean where synthetics work best, either MODAS or ISOP, are where there is strong steric variability, which generally requires stratification. If the ocean is truly unstratified, as is often the case at high latitude, there will be little SSH variability and therefore nothing for the synthetics to replicated. In this case the synthetics will simply return the climatological profile. What we are finding is that the ocean and/or our Nature run is disagreeing with our climatology

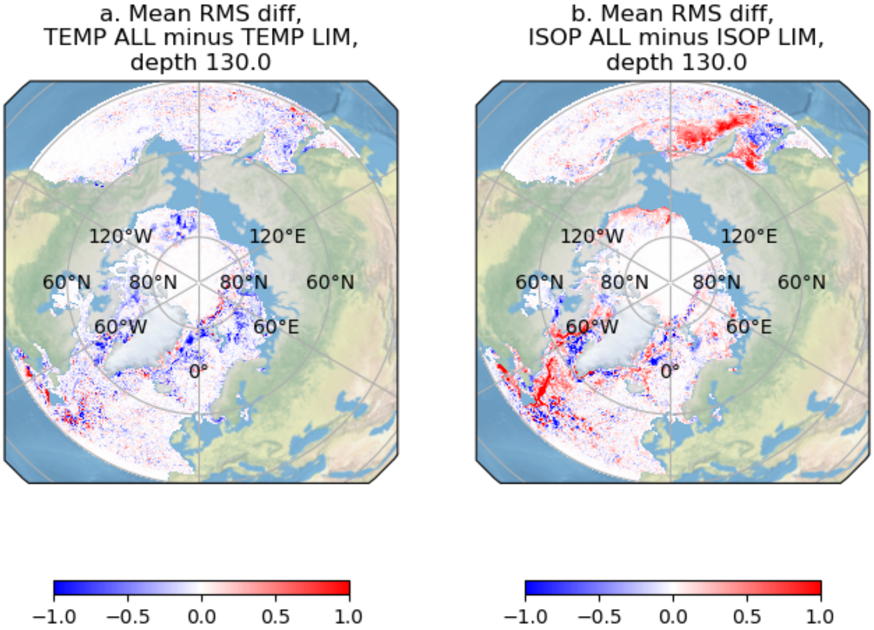

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FIG. 3. RMSD was calculated between each OSSE and the Nature Run. Shown is the difference in RMSD between a. TEMP ALL and TEMP LIMITED (where blue, indicates that TEMP ALL has a lower RMSD than TEMP LIMITED) and b. ISOP ALL and ISOP LIMITED (where blue, shows that ISOP ALL has a lower RMSD than ISOP LIMITED).

and covariances. In this case, where the ocean has a different structure from our climatology, the synthetics have trouble replicating the ocean. This problem is exacerbated at high latitude where in situ observations are sparse and the ocean has a weak steric signal. The methods for ISOP have a better chance of returning accurate results, compared to MODAS, because the SSHA constraint requires the synthetic to have steric height to match the input SSHA (see part II of this paper).

To help identify where synthetics may fail we apply the Tcheck. This requirement is implemented in ISOP LIMITED by ensuring that the temperature at 1000 m is at least three degrees colder than the temperature at the surface. This check, therefore, is designed to identify regions where there is no thermosteric signal for the synthetics to replicate. The climatology, and the associated covariances, must accurately associate a given change in sea surface height with an associated change in subsurface structure. If the climatology does not accurately depict the water structure, then using that climatology to predict water structure will be ineffective. There is no way to "check" the latter condition, and one of the risks of using synthetic profiles at high latitudes, given the rapid changes in ocean structure associated with climate change especially at high latitudes, is that the climatology will be outdated. The present analysis examines whether this is happening in some locations

b. Regional analysis

1) Temperature and Density Thresholds

To determine where ISOP could effectively be applied and what conditions prevent its use, we will focus on two specific regions, in which RMS difference maps indicate using ISOP has a strong impact. First we examine the Labrador Sea. Figure 4 shows the difference in RMS between ISOP ALL and ISOP LIMITED. In the Northern Labrador Sea, it is evident that using ISOP has a strong, positive effect. However, in the southern Labrador Sea, using ISOP evidently affects the ocean state estimate negatively. To understand what is happening here, it is necessary to examine the subsurface structure of all the information: the OSSEs, the Nature Run, and the climatology. Rather than look at a single gridpoint, a box is drawn around the region (as shown) and all profiles within that box on a single day (Dec 31, 2017) are combined into a mean profile. The boxes differ as the horizontal grids for the OSSEs, the Nature Run and the climatologies are not the same. The profiles shown in Figure 5a and b are temperature and salinity (respectively) from the northern box (Box 1 in Fig 4), and Figure 5c and d are from the southern box (Box 2).

The first thing to note is that neither of these locations have what would be considered a typical midlatitude temperature structure (warmest temperatures at the surface, decreasing with depth). In the northern box, surface temperature is significantly colder than the temperature at 1000 m. Stratification is controlled by salinity, with much fresher (and lighter) water at the surface. While the profile here fails Tcheck, it is clear that there is a distinct subsurface structure that is relatively well-represented by the climatology. The cyan "ISOP ALL" profiles more closely matches the strong increase of temperature in the first 150 m seen in the Nature Run, indicating that using ISOP improved the estimate over excluding it in this case. In the Southern Box, the Nature Run shows a similar structure, albeit with somewhat smaller amplitude. The climatology, however,

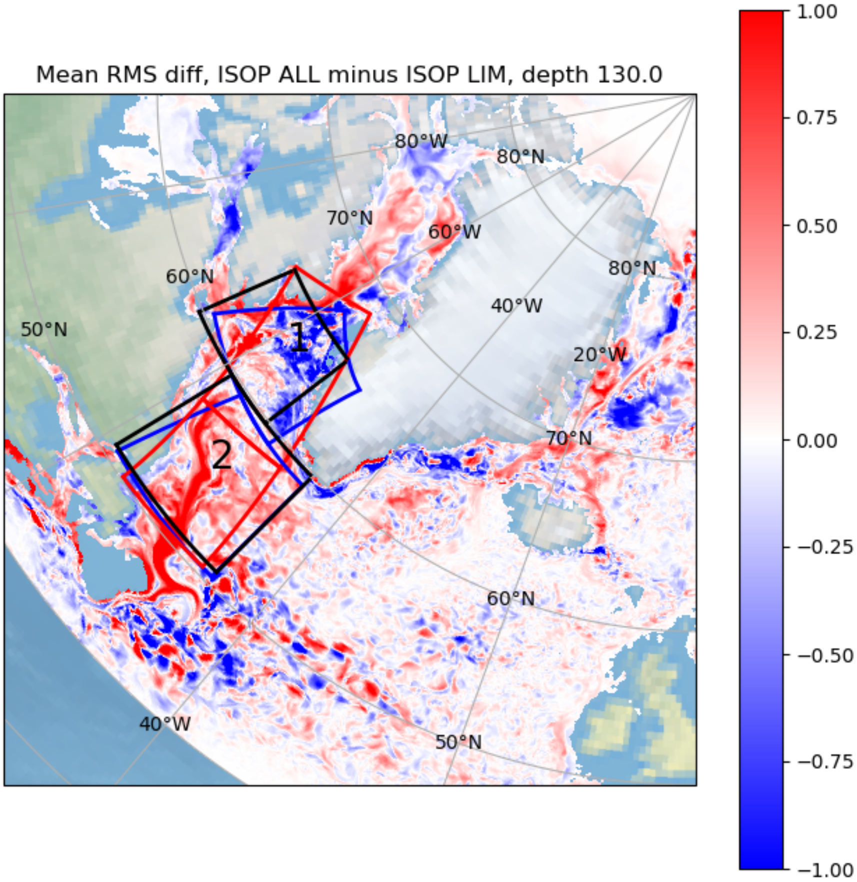

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FIG. 4. This figure shows the difference between ISOP ALL and ISOP LIMITED RMS differences in the Labrador Sea. Numbered boxes indicate regions where mean profiles were calculated from the OSSEs and the Nature Run and compared with climatology

indicates nearly constant temperature in the top 1000 m. As noted previously, ISOP performs best in a region where steric variability is strong; thus, the expectation would be poor results from ISOP. The adjustments made to the OSSE profile where ISOP is applied exacerbate the mismatch between the model and the Nature Run, as the profile is adjusted to be more similar in structure to the climatology. The cyan profile is too cold at the surface and too warm at depth, adjusted in the wrong direction at almost every depth. When sea surface height anomaly indicates a positive

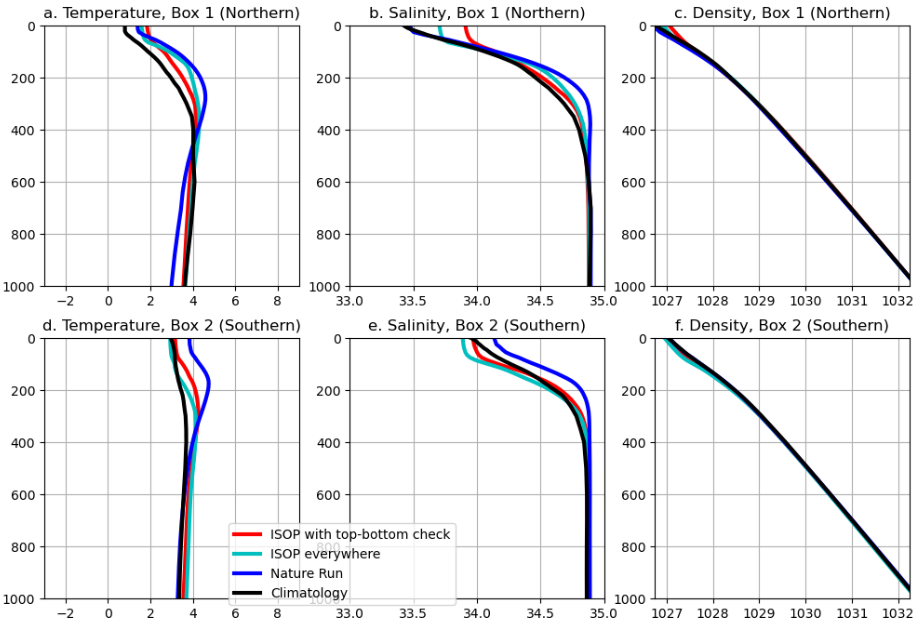

FIG. 5. Mean profiles of T, S and density in two regions of the Labrador Sea. Temperature, salinity and density in box 1 are in panels a,b and c respectively; temperature, salinity and density in box 2 are in panels d, e and f.

anomaly and the profile is unstratified, the adjustment is to warm the entire, full-depth profile. This is an example of a location where the lack of stratification means that the creation of synthetic profiles will not be able to accurately replicate the variability.

The problem is evident in this case only because we are using a Nature Run and therefore the profile we should create is known. When using the assimilative model in the real world, how can we determine whether a profile will be accurately synthesized, without knowing the true ocean state? To determine the efficacy of the "Tcheck" approach, where temperature change is the metric used to determine whether a profile can be synthesized, we evaluate the relative accuracy of the synthetic profiles as a function of Tcheck, the temperature change between the surface and 1000 m. Given the impact of salinity on stratification at high latitudes, we also evaluate the accuracy of synthetic profiles as a function of change in density. These assessments will demonstrate whether a simple threshold is the best way to determine whether a profile should be discarded. Figure 6 shows the results of these evaluations within the Labrador Sea region. In Figures 6a and 6b, we see the

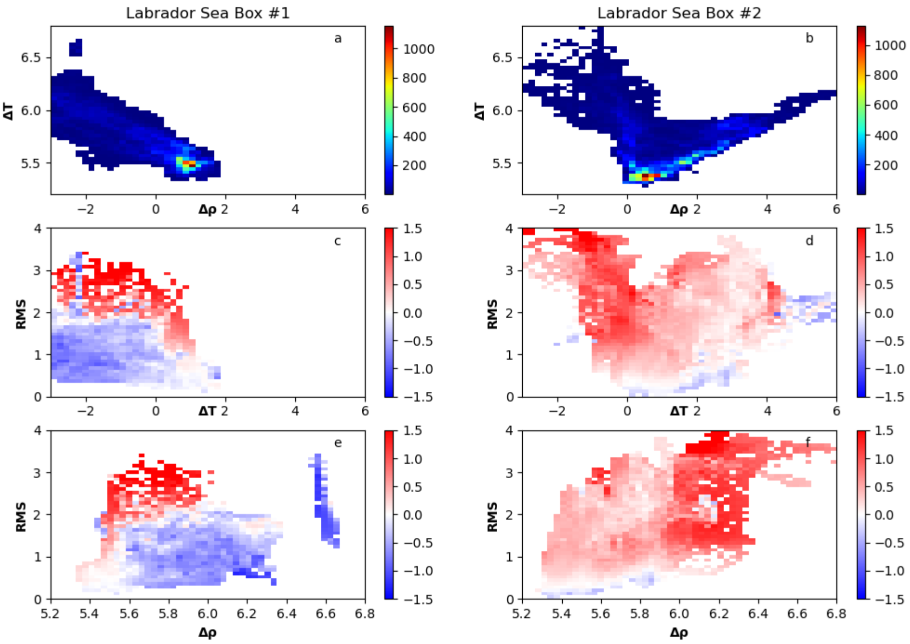

Fig. 6. Relationship between temperature change, density change, and RMS values in the Labrador Sea. a. PDF of profiles in $\Delta\rho$ and ΔT space in Northern Labrador Sea box. b. Same as a, but for Southern Labrador Sea box. c. RMS of profiles in Northern Labrador Sea box as a function of ΔT, colored by the RDIFF seen in Figure 3. d. Same as c, but for Southern Labrador Sea Box. e. RMS of profiles in the Northern Labrador Sea Box as a function of $\Delta\rho$, colored by RDIFF. f. Same as e, but for Southern Labrador Sea Box

histogram of occurrences of changes in density and changes in temperature. The largest changes in density are associated with large, negative changes in temperature, where deep temperatures are as much as 3 degrees warmer than surface temperatures. The minimum density changes occur close to temperature changes of one degree C, with density changes around 5.3 to 5.5 kg/m^2, and it is in this range that most of the profiles are located.

Figures 6c and 6d show the relationship between temperature change (x-axis) and average RMS difference between model profiles and the associated nature run profiles (y-axis). The color indicates the RDIFF as defined previously. In 6c, there is no obvious correlation between RMS values and temperature. The profiles where using ISOP gives worse results are those where the results were poor (high RMS) to begin with. It is noteworthy that there were no points in this region where the change in temperature exceeded even 2 degrees; if Tcheck were applied, none of these data would be assimilated. In 6d, the results are less straightforward. In general, it does not appear that using ISOP decreases RMS, except for a small collection of points where DeltaT is greater than about 5. The largest error increases come in the areas where errors were large to begin with, in areas where the temperature stays nearly the same or slightly increases with depth. This aligns with what we saw in the Figure 5: at locations with very small temperature changes, the ISOP-adjusted profile is shifted along its full depth. While the Nature Run shows a hint of structure, the climatology on which the ISOP profiles are built does not replicate that.

Figure 6e and 6f are similar to 6c and 6d, but use density change instead of temperature changes. Given that ocean stratification is controlled by density rather than either temperature or salinity, is there a minimum density change that should be required in order to use ISOP? In both regions (Figures 6e and 6f), the RMS differences between the run and the nature run increase with larger density changes; minimum RMS values are found at minimum density changes of around 5.4 kg/m^2. There is also no indication that use of ISOP is beneficial at higher density changes, and indeed in Box 2 (Figure 6f) the largest deficiencies in ISOP are found at the largest top-to-1000 density changes. These figures dispel the notion that a threshold of either temperature change or density change will predict whether ISOP should be applied or not, at least in the Labrador Sea region.

Next, we consider the northern Pacific, specifically the Bering and Okhotsk Seas. Three boxes are drawn in Fig 7. Box 1 is in the Okhotsk Sea, while boxes 2 and 3 are in the Bering Sea, geographically close but on the eastern side of the Kamchatka peninsula. The Okhotsk Sea (Fig 8a-b) shows a region where applying ISOP seems to improve the results, but the opposite is true in the Bering Sea (Fig 8d-i) . As in the Labrador Sea, the mean profiles of each location in the box on Dec 31, 2017, will be examined. Here, only the first 600 m are shown. In the Okhotsk Sea, while surface temperature and temperature at 600 m are similar, there is a temperature minimum at about 100 m that is well-defined and shown in the climatology, the Nature Run, and the ISOP ALL profiles. The ISOP LIMITED profile does not have this feature. This is an indication that ISOP should be used here; it is clear that using it brought the results much more closely aligned with the actual ocean state. However, in the Bering Sea, the results tell a different story. The climatology still has a strong temperature minimum at 100 m, and the ISOP ALL results match that feature. However, in this case, the feature is not seen in the Nature Run. The structure of the

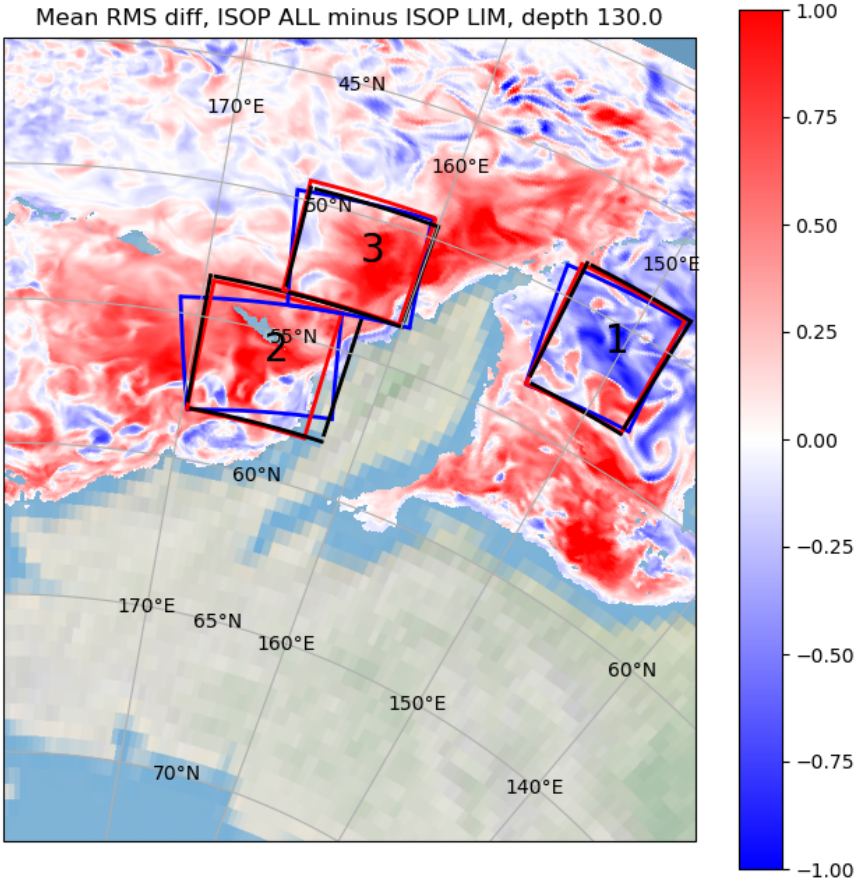

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FIG. 7. This figure shows the difference between ISOP ALL and ISOP LIMITED RMS differences on the Pacific side of the Arctic regions. Numbered boxes indicate locations in the Okhotsk Sea and in the Bering Sea where mean profiles were calculated from the OSSEs and the Nature Run and compared with climatology.

ISOP LIMITED profile is quite close to the structure seen in the Nature Run. The implication here is that the disconnect between the climatology and the Nature Run is causing the method to give inaccurate results. The ISOP system is constrained by climatology, so when it is applied the profile is adjusted to include features like the subsurface minimum. This is a situation where without the correct climatology, nothing can truly be done to correct the situation.

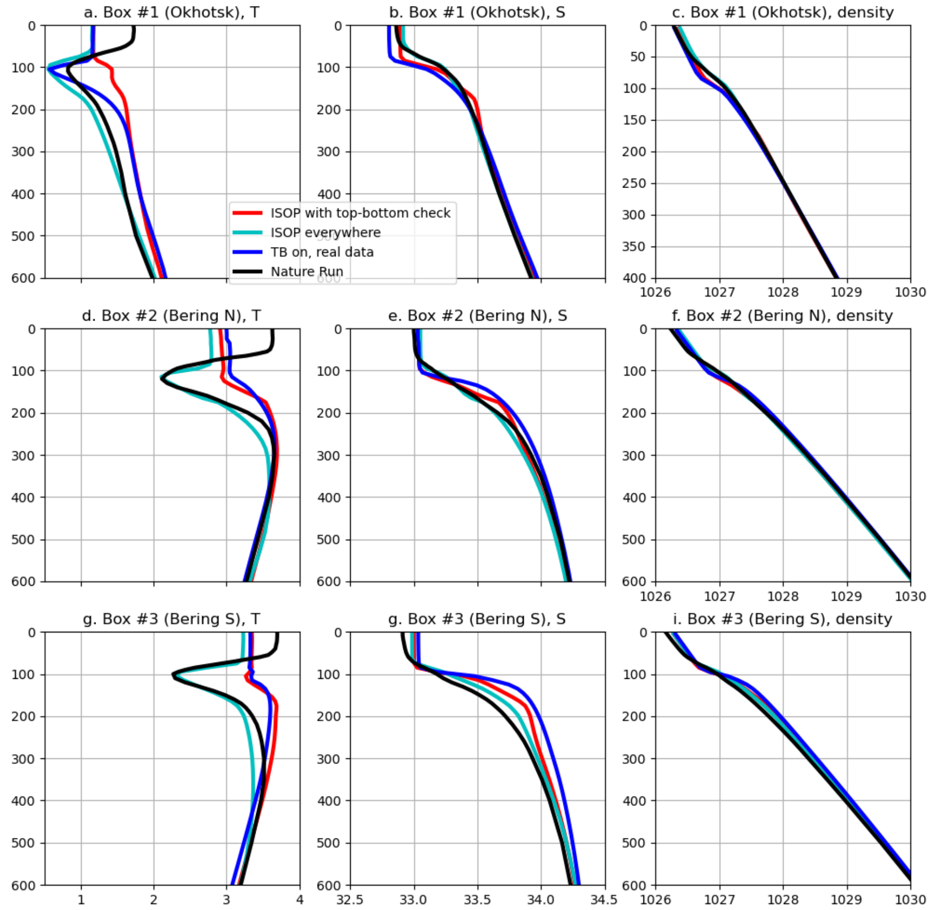

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Fig. 8. Profiles averaged over regions for Dec 31, 2017. Regions shown in Figure 7. a. Okhotsk Sea, temperature; b. Okhotsk Sea, salinity; c. Okhotsk Sea, density ; d. Bering Sea region 2, Temperature; e. Bering Sea region 2, salinity; f. Bering Sea region 2, density; g. Bering Sea region 3, temperature; h. Bering Sea region 3, salinity; i. Bering Sea region 3, density.

Given the noted discrepancies, would a threshold method have worked to determine whether to apply ISOP in this region? We proceed with an analysis of RMS as a function of ΔT and $\Delta\rho$ as for the Labrador Sea. Figure 9 uses the same axis limits as Figure 6. The profiles in these regions have much smaller ranges of variability; all have relatively high $\Delta\rho$ of more than 6 kg/m^2. Most profiles in the sea of Okhotsk have ΔT below 0, and the blue color demonstrates that most profiles

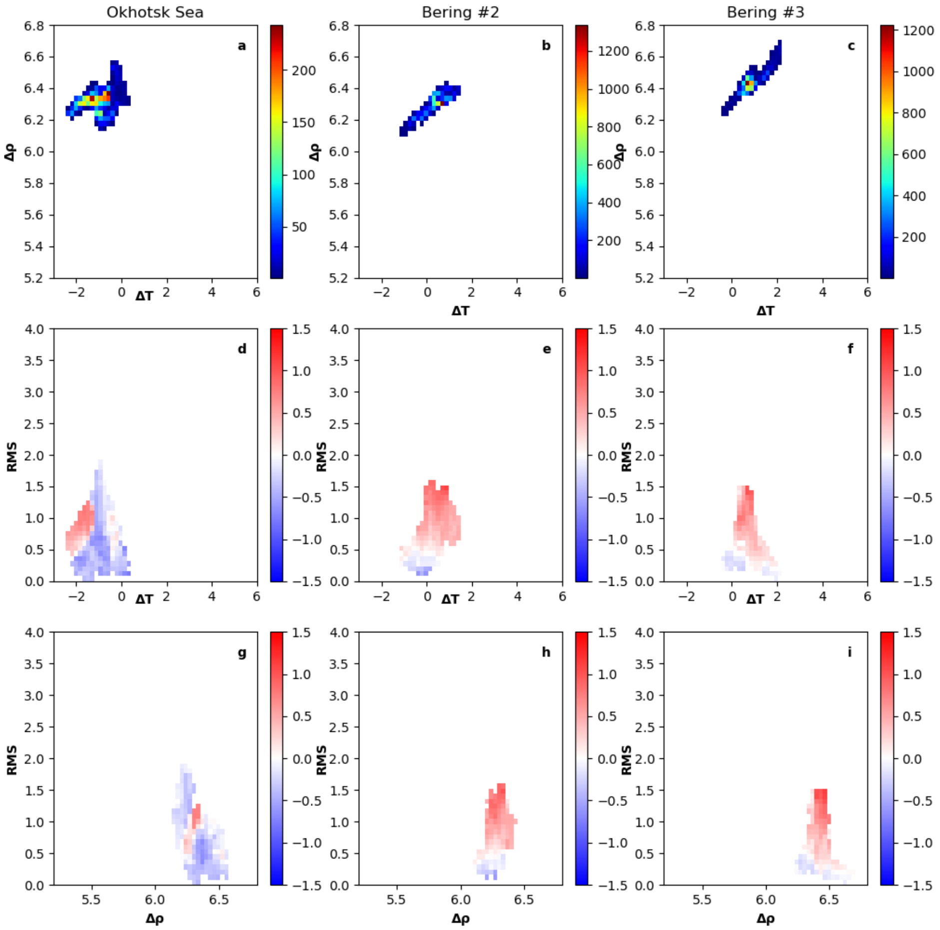

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Fig. 9. Relationship between temperature change, density change, and RMS values in the Northern Pacific. a. PDF of profiles in $\Delta\rho$ and ΔT space in Okhotsk Sea box. b. Same as a, but for Bering Sea box 2. c. Same as a, but for Bering Sea box 3. d. RMS of profiles in Okhotsk Sea box as a function of ΔT, colored by the RDIFF seen in Figure 3. e. Same as d, but for Bering Sea Box 2 f. Same as d, but for Bering Sea Box 3. g. RMS of profiles in the Okhotsk Sea Box as a function of $\Delta\rho$, colored by RDIFF. h. Same as e, but for Bering Sea Box 2 i. Same as e, but for Bering Sea Box 3

are better simulated with the use of ISOP. The profiles in the Bering Sea have ΔT centered on zero, and are mostly not well simulated by ISOP, as shown in Figure 8. There is no obvious correlation between ΔT and RDIFF, nor between $\Delta\rho$ and RDIFF. For the analysis of RMS and RDIFF based on $\Delta\rho$, the three regions all have similar $\Delta\rho$, also similar RMS differences between the results and the Nature Run, but the changes in RDIFF indicate that the use of ISOP is uncorrelated with any of these factors.

2) T-S RELATIONSHIPS

Since neither a temperature or density change threshold can predict as to whether ISOP can be used, we need to consider the problem from a different perspective. One possibility is to consider the problem in terms of water mass properties and deviations from the mean. The climatology and covariances are constructed from in situ data and thus comprise the variability of the water mass most likely to reside in a given region. The water mass is described not by temperature alone (as assumed in Tcheck) but also by salinity, and their deviations from the mean. To examine this, we plot the histogram of ΔT vs ΔS, to determine what T-S relationship is represented in a specific region. First, we consider the Labrador Sea. Figures 10a and b show the PDF of ΔT vs ΔS. In both the northern and southern regions, most of the profiles have roughly the same ΔS-ΔT relationship, with ΔS close to 1 and a ΔT between -0.5 and 0. Then we plot the average RMS value of all profiles at each T/S intersection, letting us know whether profiles with a given T/S relationship are well-represented by ISOP or not. Note that this represents the difference between ISOP ALL and the Nature Run, rather than the RDIFF quantity presented in earlier figures. The profiles in the ΔT/ΔS range where most profiles are located have generally lower RMS values; if a profile is within the "normal" range for the T-S water mass generally present in the region, than the synthetic profile gives a relatively good match to the Nature Run profile. This indicates that the way we determine whether a profile will be well-represented is not based on density, or even on stratification. By examining the T/S relationship of a profile, we can determine whether it is within a range that will be reasonably likely to have a low RMS value. The final two panels of Figure 10e and f show the RDIFF value as a function of ΔT and ΔS. It is obvious that the T-S ranges where most profiles exist are improved by using ISOP ALL rather than ISOP LIMITED. These regions are white to very light red, indicating a neutral response to slight degradation of results from using ISOP. Additionally, the range of ΔT/ΔS where ISOP ALL is advantageous in the northern Labrador Sea box has slightly smaller ΔS for the same ΔT as those regions where ISOP ALL is disadvantageous in the southern Labrador Sea box, indicating that these ranges can be used to delineate guidelines for when ISOP ALL should be applied. (Part II of this paper will continue to examine this relationship under a different framework, which does not involve the Nature Run in the same way.)

We can examine this relationship in the Pacific region as well. In the Okhotsk Sea, we find again that the locations where most profiles are located have low RMS values, but there is a lot more spread in the ΔT-ΔS relationship (11a and b). Examining Figure 11g, we see that in these locations, ISOP ALL is a clear improvement over ISOP LIMITED. The profiles in the Bering Sea are located in a tight ΔT-ΔS range, with larger ΔS and smaller ΔT than the Okhotsk Sea (Figures 11b,c,e, and f. In both cases, the Bering Sea values are concentrated in regions where RMS is high, and where ISOP LIMITED provides advantages over ISOP ALL (FIgures 11h and i); we have previously discussed this issue as a reflection of the mismatch between the Nature Run and the climatology. However, the ΔT-ΔS diagram can be used to exclude the Bering Sea profiles and include those in the Okhotsk Sea, by indicating the range of ΔT-ΔS considered acceptable. This could be a relatively simple metric that would allow us to include or exclude profiles based on whether ISOP has shown skill in accurately synthesizing profiles in the water mass under consideration.

As we have focused our analysis on two very specific regions, we should acknowledge that the application of a metric such as this may not be as simple as it first appears. The advantage of pursuing this approach is that it allows us to define a metric that assesses the applicability of ISOP that is based on the physical properties of the ocean, and rooted in a quantitative assessment of success, rather than an arbitrary threshold, especially since we have demonstrated that the threshold approach is of limited utility. One would expect the water masses in which ISOP has success to vary spatially, much as the water masses present in the ocean have strong spatial variability. In order to assess the viability of this approach, we look at the ΔT/ΔS diagrams for the full Atlantic and Pacific Oceans (north of 40°N, which is the extent of the OSSE region).

In Figure 12a we see the histogram of profiles in the Atlantic Ocean as a function of ΔT and ΔS, and it is clear that most of the profiles do lie within a relatively small range of variability. In Figure 12c, we see that within that small range of variability, the resulting RMS values tend to be small. Thus, while there is not a cutoff for ΔT or ΔS that will ensure profile quantity, there is a range of ΔT/ΔS that will provide the metric we need. The results in the Pacific are less clear-cut, but we can still see that there is relatively low RMS in the range of variability where most data are found.

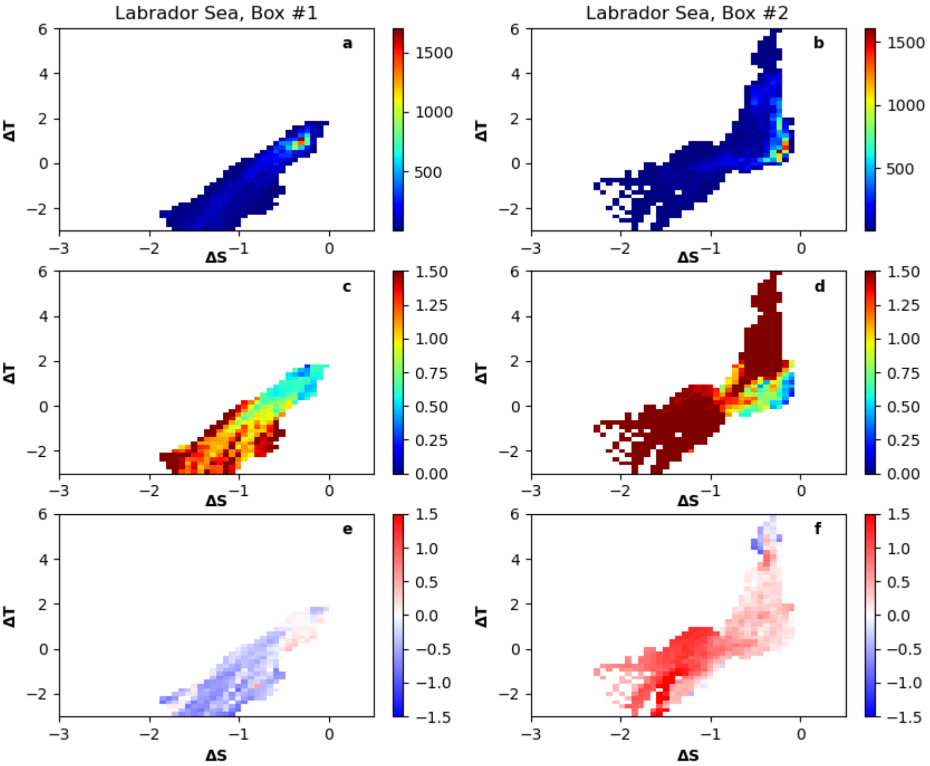

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FIG. 10. Relationship between ΔT and ΔS in the Labrador Sea. a. PDF of profiles in ΔT and ΔS space in Northern Labrador Sea box. b. Same as a, but for Southern Labrador Sea box. c. Average RMS of profiles in Northern Labrador Sea box at each ΔT/ΔS location. d. Same as c, but for Southern Labrador Sea Box. e. Average RDIFF of profiles in the Northern Labrador Sea box at each ΔT/ΔS location. f. Same as e, but for the Southern Labrador Sea.

We can also see that the range of variability in the Pacific is different than the Atlantic, so there will need to be spatial variability included in this metric; however, it does appear that we can think of this as varying on the scales of full ocean basins; fine resolution will not be necessary. Finally, Figures12e and f demonstrate the range of regions in which ISOP ALL improves the solution. Together, these figures can provide a guide toward determining where ISOP should be applied and the confidence the user should have in its accuracy (which could be use to adjust weights when assimilating these synthetic profiles). This premise will be examined more fully in Helber et al. (2024).

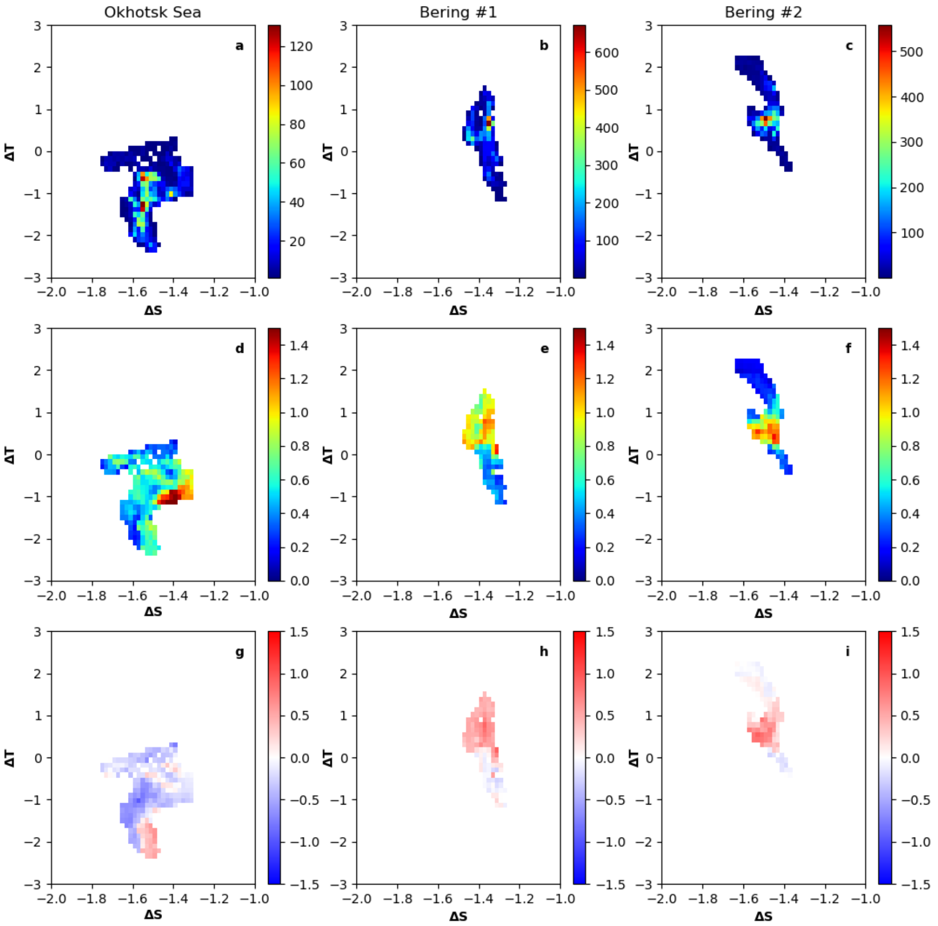

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Fig. 11. Relationship between ΔT and ΔS in the Pacific Ocean. a. PDF of profiles in ΔT and ΔS space in Okhotsk Sea box. b. Same as a, but for Northern Bering Sea box. c. Same as a, but for Southern Bering Sea box. d. Average RMS of profiles in Okhotsk Sea box at each ΔT/ΔS location. e Same as d, but for Northern Bering Sea Box. f. Same as d, but for the Southern Bering Sea box. g. Average RDIFF of profiles in Okhotsk Sea box at each ΔT/ΔS location. h Same as g, but for Northern Bering Sea Box. i. Same as g, but for the Southern Bering Sea box.

5. Conclusions

In summary, four OSSEs were performed to analyze the performance of current assimilation methods at high latitudes. These OSSEs are intended to analyze the impact of assumptions in

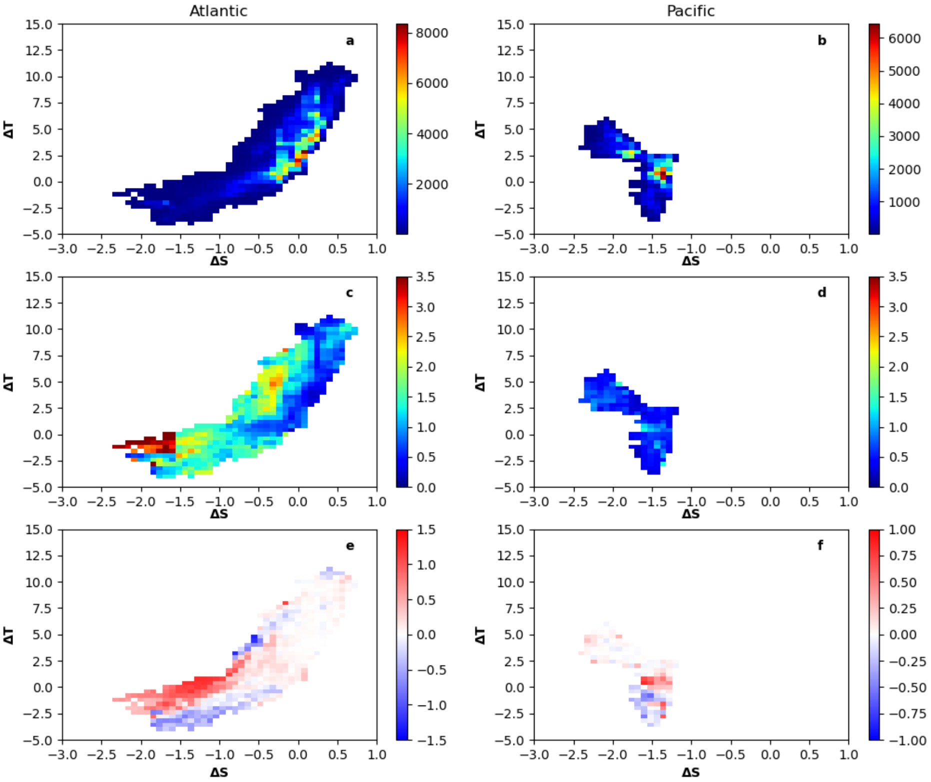

FIG. 12. a. PDF of profiles in ΔT and ΔS space in all Atlantic locations north of 40°N. b. Same as a, for Pacific locations north of 40°N. c. Average RMS of profiles in Atlantic locations north of 40°N in ΔT and ΔS space. d. Same as c, for Pacific locations north of 40°N. e. Average RDIFF for all locations in Atlantic north of 40°N in ΔT and ΔS. f. Same as e, for Pacific locations north of 40°N.

the currently used assimilation framework. The first assumption being tested is the metric of temperature difference between the surface and 1000 m depth as a metric for stratification. This assumption results in a large amount of satellite sea surface height data being discarded, rather than used in the assimilation process. By assimilating the actual temperature profiles at these locations, we can determine how much our results would be improved if we could accurately use these data to estimate temperature profiles, as is done in more stratified locations. The conclusion here is that there is nearly no basis for a threshold of either temperature or density to be used as the basis of determining the applicability of ISOP. The relationships between ΔT and $\Delta\rho$ and the RMS between the profiles and the Nature Run show no correlation, and therefore the idea that this could be used as the determining factor is faulty. However, we find that there is a relationship between the RMS of profiles and the ΔT/ΔS relationship. When ΔT and ΔS are both used, their intersection can provide a location where the ISOP profile can be assumed to be accurate or inaccurate. The physical explanation is that ISOP does well at characterizing the variability of certain water masses, and if the profile is within those bounds, it is likely to properly represent the variability. While this is not a "quick fix", and further analysis will be necessary to provide the details of the new metric, we are confident that a metric can be developed along these lines that will allow for the inclusion of much data that is currently discarded, while still excluding those profiles that cannot be accurately synthesized with the current system.

The remaining problem is the dependence on a climatology which may or may not be accurate. In this case, we are using a Nature Run, and it is straightforward to check whether the climatology "agrees" with the results. Also, the reader can refer to Helber et al. (2024) for an analysis that uses extensive observations rather that model results, but comes to many of the same conclusions found here. While the science of developing the climatologies should not be impugned, the evolution of the Arctic as the globe warms cannot be ignored, and great care must be taken to ensure that our results continue to agree with the most current observations. It is clear that if the climatology is not accurate, applying ISOP can "pull" the solution away from the correct answer instead of toward it. If we cannot obtain more observations, then we should at least evaluate those we have to see if there have been long-term shifts, and to potentially weight means toward more recent data. Assumptions that climatologies are constant are not defensible in the current changing climate. This will ensure that we are able to create accurate operational oceanographic estimates of the Arctic that reflect the true reality of the current ocean state.

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Data availability statement.

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