Section 8

Development of and advances in ocean modelling and data assimilation, sea-ice modelling, wave modeling

Inclusion of Significant Wave Height Analysis to NCEP's UnRestricted Mesoscale Analysis (URMA)

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Introduction

The National Centers for Environmental Prediction (NCEP) of NOAA provides weather guidance to the United States National Weather Service (NWS), according to the demands of our customers and the public. In this effort, two significant components of NWS operations are combined: wind-wave predictions and NCEP's UnRestricted Mesoscale Analysis (URMA). The approach is currently being developed at NCEP's Environmental Modeling Center (EMC).

From one side, NCEP's operational wave guidance products are provided at global and regional scales, within both deterministic and ensemble-based systems, e.g. [1-4]. NCEP's operational wave prediction systems are implementations of the WAVEWATCH III (WW3) model [5]. Currently the suite of operational wave systems does not include an assimilation nor an analysis component. From the other side, NCEP's Real Time Mesoscale Analysis (RTMA) [6] and its extension, URMA, both provide the highest quality gridded surface analysis. The latter systems are under continuous development to improve the analysis and, more often, to add new analysis variables to match those forecasted in the National Digital Forecast Database (NDFD) [7].

The expansion of URMA to include wave-height analyses is part of a broader effort, which aims at developing data assimilation and analysis components in NCEP's operational wave models. The project involves EMC scientists from the marine and mesoscale atmospheric branches, and its objective is to offer a new, high-resolution significant wave height (Hs) analysis product for the URMA domains to its customers and the general public.

The Wave-Height component of URMA

URMA is an extended run of the RTMA, run six hours later in order to incorporate observations that arrive after the RTMA deadline. Both are high spatial (2.5km) and temporal (1h) resolution analysis systems for near-surface weather parameters. Their main component is NCEP's Gridpoint Statistical Interpolation (GSI) system [8] applied in two-dimensional variational mode, to assimilate in-situ and satellite-derived observations. As the Hs is a two-dimensional field, the URMA may be naturally extended in order to be used for its analysis [9].

In this framework, the GSI has been updated accordingly, in order to be compatible with the requirements for Hs analysis. A module for importing altimeter Hs measurements from three satellites (Jason-2, CryoSat-2 and Saral/Altika) has been introduced, including a multi-step quality control (QC) procedure based on the signal properties themselves, but also on the expected physical properties of the wave field. For the in-situ measurements of Hs (buoys and ships), the PREPBUFR format is used, as for the majority of conventional observational data for assimilation at NCEP. For all the data a gross error check is applied. In addition, for the extension of URMA to include the Hs analysis, the GSI code has been modified to accept variance and correlation lengths that vary in both spatial dimensions: latitude and longitude.

In its initial development phase, the URMA-Wave prototype has been implemented for the coastal areas around the continental US. The background Hs is provided by NCEP's global deterministic wave model system (Multi-1), which is interpolated to the URMA grid through a combination of linear and nearest neighbor interpolation. Multi-1 is forced with GFS winds and NCEP's high-resolution ice-analyses, as described in [1]. The background and error parameters of the covariance functions have been estimated based on two years of model and buoy data. The cycling of the Hs analysis is hourly, following the cycling of the rest of the URMA variables, and uses measurements and predictions from the last 3h before the analysis.

Conclusions and Operationalization of URMA-Hs

As this is a new effort for wave data analysis and assimilation at NCEP, important groundwork was done in all components of the DA system, including standardizing the satellite altimeter data stream, developing a data quality control process, updating the GSI system, exporting and interpolating the Hs from WW3 and estimating the background and error inputs necessary for the URMA-Wave. Most of these steps will also be used in other components of a broader wave DA system which are under development, including a local ensemble transform Kalman filter (LETKF) probabilistic wave analysis and multi-dimensional variational analysis systems.

Currently, URMA-Hs runs only for the oceanic areas associated with URMA's CONUS domain, but after tests of its components and validation of the analysis, it will also be implemented for all domains distributed under the NDFD, including Puerto Rico, Hawaii, Guam and Alaska. The new URMA-Hs product is scheduled to be launched operationally with the next RTMA upgrade cycle, currently scheduled to be completed by December 2016.

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Surface heat flux corrections for Global Ocean Forecasts

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Introduction

RTOFS (Real Time Ocean Forecast System)-Global is the first global eddy resolving ocean forecast system implemented operationally at National Centers for Environmental Prediction (NCEP) in close collaboration with US Navy. It will soon be upgraded to Version 1.1. The core model and configuration were developed and validated at National Research Laboratory (NRL), using the Hybrid Coordinates Ocean Model (HYCOM) at 1/12° horizontal resolution coupled with Los Alamos Community sea ICE model (CICE). The RTOFS forecast system runs once a day and produces forecasts from the daily initialization fields produced at NAVOCEANO (NAVal OCEANographic Office) obtained using NCODA (Navy Coupled Ocean Data Assimilation), a 3DVAR data assimilation methodology (Cummings and Smedstad, 2013).

The RTOFS forecasts were developed and validated at Environmental Modeling Center (EMC). Each day, a 2-day spin up starts with the analysis of 2 days before the present, using the ocean model in forecast mode forced with hourly NCEP's Global Data Assimilation System (GDAS) atmospheric fluxes. This is continued from the present with an 8-day forecast cycle forced with 3-hourly momentum, radiation, and precipitation fluxes from NCEP's Global Forecast System (GFS) fields for the next eight days.

Following flux-corrections efforts at NRL (Metzger et al., 2013; Hogan et al., 2016), heat flux corrections are computed for the RTOFS v1.1 configuration.

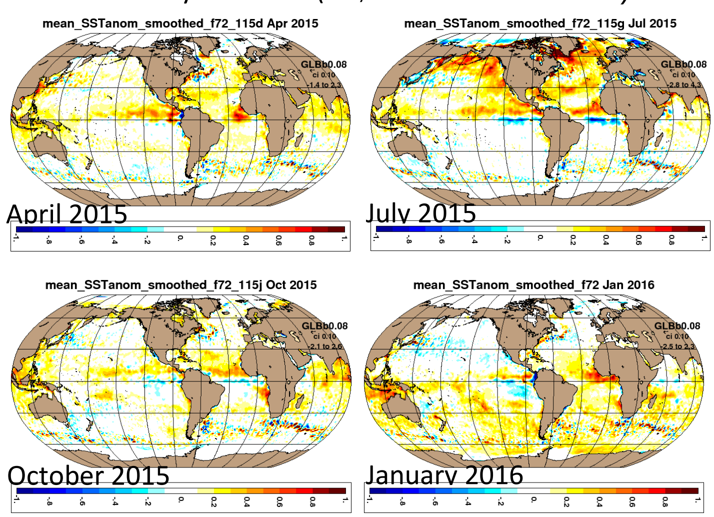
SST errors and Net heat flux corrections

Net heat corrections are computed to minimize the 5 day SST forecast error (Metzger et al., 2013; Hogan et al., 2016).

The SST error for the first 5 days of the forecast - which starts 2 days before the present - was taken as the difference between the 5 day forecast and the analysis at the date of the 5 day forecast.

SST error= SST (day 5 of forecast) – SST (analysis for day 5)

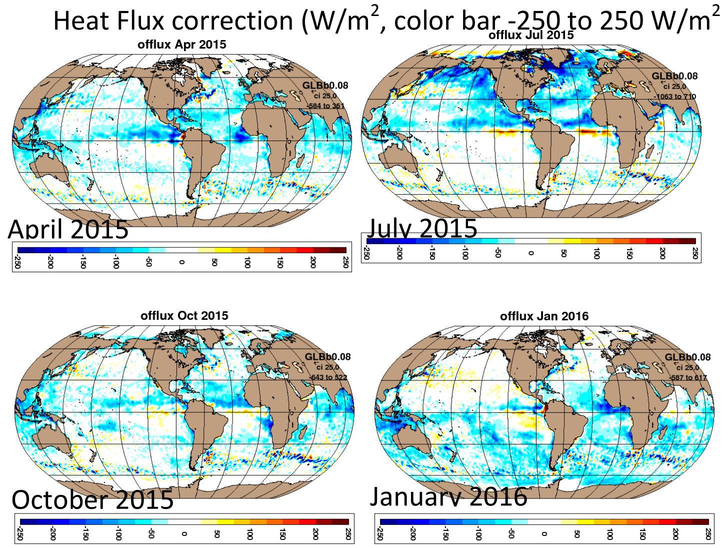
5-day SST error (°C, color bar -1 to 1°C)



The monthly mean space smoothed SST 5 day error (SST error) is converted to a surface heat flux applying a factor of -250 to the SST error to obtain the heat flux ((Metzger et al, 2013)

Net Heat Flux correction = -250W/(° m^2) * SST error

This amount of heat would, for example, cool the upper near-surface ocean by 1°C till a depth of 26m. Since this analysis was done with forecasts during March 2015 to Feb 2016, effects of the 2015-2016 El Niño and others can be present in the correction fields. Flux correction estimates when applied will be based in SST errors from previous years/months; therefore, this method does not minimize the error for a particular year/month.



The correction should compensate for a warm SST error in the summer hemisphere (Southern hemisphere for January and Northern hemisphere for July), which was found to be present in several years. The warm narrow band north of the equator and cool band south of it was seen in other years, but its details may vary.

The following comparisons with other years/products were done:

a) Hogan et al. (2016)'s 5-day SST errors with GDAS for 2014 show generally consistent patterns.
b) Forecasts done with next future upgrades for GDAS/GFS (available as a parallel GDAS/GFS run) result in small differences for flux corrections.

Simulations with flux corrections are being performed. Metzger et al. (2013) demonstrate an improvement in the SST error when the same simulations from which the flux corrections were obtained are redone with flux correction. When the flux correction obtained in a year is applied to simulations from other years it is to be expected that the improvement will be diminished. In addition to flux corrections, residual flux corrections will be computed and applied if necessary.

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Simulated global HYCOM (GLBa0.24) results from various ocean color forcings: Preliminary results from sensitivity analyses

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Chlorophyll *a* (Chl-*a*) is one of the most commonly used biomass indicators in marine phytoplankton ecology. Phytoplankton are primary producers of organic materials, and in the upper ocean, have their own internal physical and biogeochemical (BGC) dynamics. Along with photosynthesis, another major aspect of phytoplankton in the upper ocean is their role in attenuating radiant fluxes through optical processes such as absorption and scattering. Chlorophyll *a* and its attenuation characteristics can be estimated through remote sensing techniques. Despite the reality that observations are limited to 2-dimensional surface fields, remotely-sensed ocean color data (Chl-*a* concentration and the diffuse attenuation coefficients at 490 nm (K_{d490}) and for photosynthetically available radiation (K_{dPAR})) have been by far the most easily accessible and most frequently used products for providing an up-to-date state of marine primary producers (phytoplankton) and their photosynthetic activity (primary production). This bottom-up control is critical to understanding the dependent oceanic food webs in a region and the biogeochemical cycles relevant to global processes. In addition, data assimilation of ocean color products (e.g., SeaWiFS, MODIS, VIIRS) will provide a unique and timely opportunity to establish a path toward ecological forecasting through biogeochemical analyses and forecasts.

As a component of initial efforts to test operational feasibility and capability, we investigated the effects of various ocean color products on ocean model behaviors and its upper ocean thermal structure. We used a 1/4^o Hybrid Coordinate Ocean Model (HYCOM; GLBa0.24 hereafter) with cylindrical (78.64°S – 66°S); recti-linear coordinate (66°S – 47°N); and. Arctic bipolar patch (>47°N). It has vertical coordinates employing 32 layers with following isopycnals in the deep sea, z-levels in the surface and a terrain-following σ-coordinate near coastal areas [1]. K-Profile Parameterization (KPP) [2] is used as a vertical mixing scheme. GLBa0.24 was forced by hourly atmospheric fluxes from NOAA's Climate Forecast System Reanalysis (CFSR) [3]. Four numerical experiments were set up by combining three different ocean color products and two shortwave radiant flux algorithms (Table 1).

Table 1. Various ocean color products used by RTOFS-Global for short wave radiant fluxes.

Experiments	Ocean color product	Sensor	Period	Algorithms
KparCLM	Long-term climatological K_{dPAR} [4]	SeaWiFS	1997-2010	[5]
ChlaCLM	Long-term climatological Chl-*a* [6]	SeaWiFS	1997-2010	[7]
ChlaIND	Interannual mean Chl-*a* [6]	SeaWiFS	Each year (2001 – 2010)	[7] with no diurnal variation
ChlaID	Interannual mean Chl-*a* [6]	SeaWiFS	Each year (2001 – 2010)	[7] with diurnal variation

KparCLM is based on a 13-year long-term climatological K_{dPAR} derived from SeaWiFS [4]. The algorithm to compute shortwave radiant fluxes is based on K_{dPAR} [5]. ChlaCLM is based on a 13-year long-term Chl-*a* derived from SeaWiFS [6] and the shortwave radiation algorithm used in this experiment directly uses Chl-*a* to compute inherent (*a*: absorption coefficients) and apparent optical properties (K_d: downwelling attenuation coefficient; θ: solar zenith angle) [7]. ChlaIND and ChlaID use the same ocean color forcing, interannual mean of SeaWiFS Chl-*a* but the former experiment does not consider the diurnal effects of solar zenith angle, whereas the latter included diurnal changes of the Sun's incident angle (0^o to 60^o as described in [7]). In summary, the comparison between KparCLM and ChlaCLM gives algorithmic differences; the comparison between ChlaCLM and ChlaIND gives effects of mesoscale variabilities; and the comparison between ChlaIND and ChlaID yields diurnal variabilities and short-term scale effects. All experiments were initialized at January 1, 2001 and ran for 10 years. Surface temperature values are not constrained to data (no surface relaxation to climatology).

Figures 1 and 2, respectively, represent a snapshot of differences in sea surface height (SSH) and sea surface temperature (SST) between the experiments one year after the initialization. Differences are noticeable in the areas of surface boundary currents, such as Kuroshio Current, Gulf Stream, Benguela Current, and Antarctic Circumpolar Current. The Equatorial Pacific also revealed basin-wide noticeable changes in both SSH and SST. It is noteworthy that the algorithmic difference (Figs.1a and 2a) created larger scale changes compared to other comparisons (e.g., changes in SSH in the Southern Ocean area; basin-wide changes in Pacific Ocean SST). Although it is apparent that the sensitivity of different ocean color products and optical algorithms made noticeable changes, more robust statistical analyses are required to confirm these synoptic findings in the comparisons.

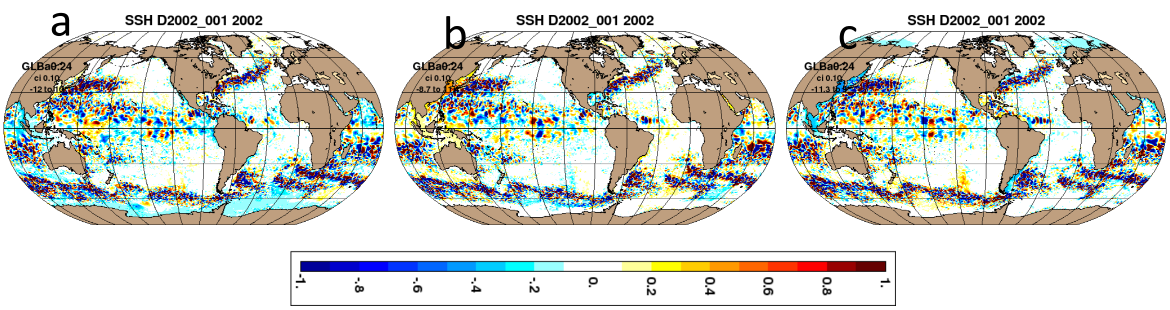

Fig. 1. Differences in SSH between KparCLM and ChlaCLM (a); ChlaCLM and Expt03.2 (b); and ChlaIND and ChlaID (c).

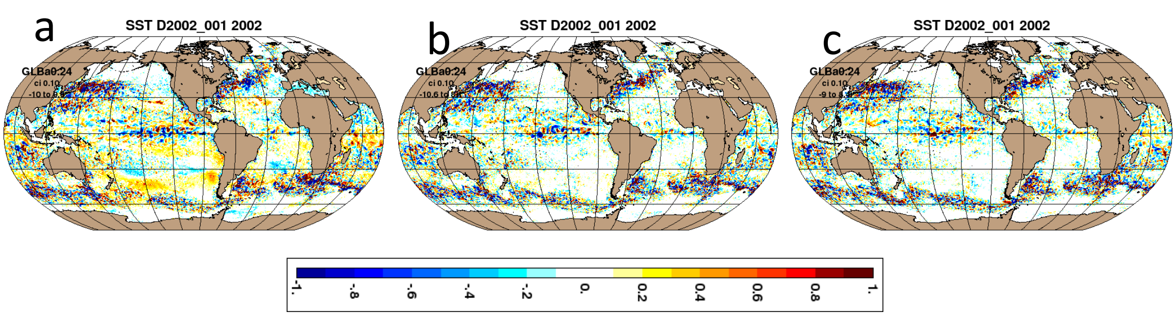

Fig. 2. Differences in SST between KparCLM and ChlaCLM (a); ChlaCLM and Expt03.2 (b); and ChlaIND and ChlaID (c).

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Consistent Ocean Color and its Assimilation in Ocean Models

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Satellite remote-sensing of ocean color (OC) parameters provides a means for broadly observing the foundation of the biological component of the world's oceans. Consequently, this data needs to be exploited for the analysis and prediction of ocean bio-physical processes and initiating the biogeochemical path, through primary productivity and associated processes and natural cycles, to ocean ecological forecasts. Operational integration/assimilation of OC fields (chlorophyll, Kd490, KdPAR) into NOAA's operational ocean models has three fundamental requirements/conditions: 1) gaps in the observations need to be addressed, both in the current instance and for extended gaps; 2) the data being assimilated must have a long data record for establishing a robust statistical database that spans multiple seasons; and 3) for assimilation, the data must be for a predicted parameter.

In previous work [1], we demonstrated that a neural network (NN) technique can successfully fill both short and small gaps (several days and several grid points), as well as extended gaps (several months and global) in satellite OC measurements. In this work, we show that the other two principal requirements can also be satisfied using the NN technique.

Consistent Ocean Color

Three major OC data sets exist, produced by the SeaWiFS (09/1997 – 12/2010), MODIS (07/2002 – present), and VIIRS (1/2011 – present) sensors. These three data sets have different error statistics; therefore, it is not a simple task to integrate them into a single consistent long-term data set. One possible approach is examined here. Using three years of VIIRS data (the most accurate and recent measurement), we trained an ensemble of NNs. Each of the NN ensemble members performs a mapping of relevant ocean variables (SST, SSH, and the upper-ocean portions of vertical temperature and salinity profiles) to the logarithm of chlorophyll-a concentration, *C*, which can be expressed as:

$$LC = \log_{10} C = NN(SST, SSH, \vec{T}, \vec{S}, lat, lon, doy) \tag{1}$$

where $\vec{T}$ and $\vec{S}$ are the upper-ocean portions of the temperature and salinity profiles, and *doy* is the day of the year. Using a logarithm of C as the NN output, rather than C, produces a more accurate NN approximation and extrapolation of VIIRS data. When training the NNs, the mean square error function is used; however, this error function is optimal for normally distributed data. Chlorophyll data have an almost log-normal distribution (see Fig. 1); thus, $\log_{10} C$ is nearly normally distributed (Fig.1). Using three years of VIIRS data for training with $\log_{10} C$ as the NN output produced an ensemble of NNs capable of stable long-range extrapolation of chlorophyll values.

For signatures of upper-ocean dynamics this study employs satellite-derived surface variables (sea-surface temperature (SST), sea-surface height (SSH)), and gridded ARGO salinity and temperature profiles of the top 75m depth. Chlorophyll fields from NOAA's operational Visible Imaging Infrared Radiometer Suite (VIIRS) are used. The NNs are trained using data for three years (2012 through 2014) and assessed for a period of 10 years (2005 through 2014). To reduce noise in the data and to obtain a stable computation of the NN Jacobian for sensitivity studies and data assimilation [2], an ensemble of NNs was constructed. Results are assessed using the

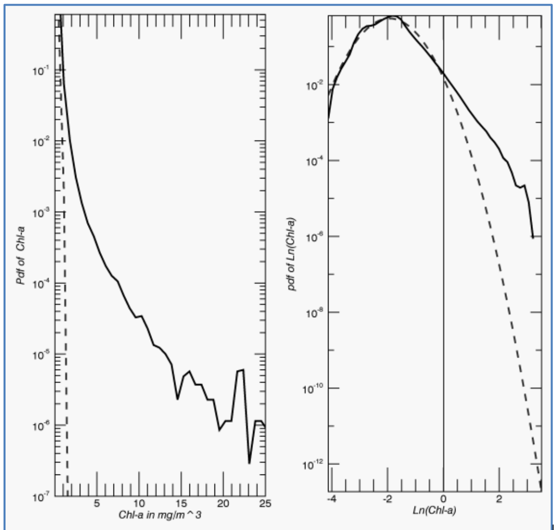

Fig.1 Probability density function for C (left panel and for $\ln C$ (right panel) shown by solid lines. In both panels, dashed lines show normal distribution with the same means and standard deviations.

root-mean-square error (RMSE) metric and cross-correlations between observed chlorophyll fields and NN output. Chlorophyll measurements from the three different OC sensors (SeaWiFS, MODIS, and VIIRS) available during the validation period were used. Fig. 2 presents the validation results. The correlations between the NN-generated and observed C decrease slightly from ~0.85 to ~ 0.75 when moving away from the training interval (2012 through 2014). RMS differences, however, do not change significantly. Results for all three used satellite sensors are very consistent. It means that NN generated C can serve as consistent long term OC data for different uses, including assimilation in to ocean models.

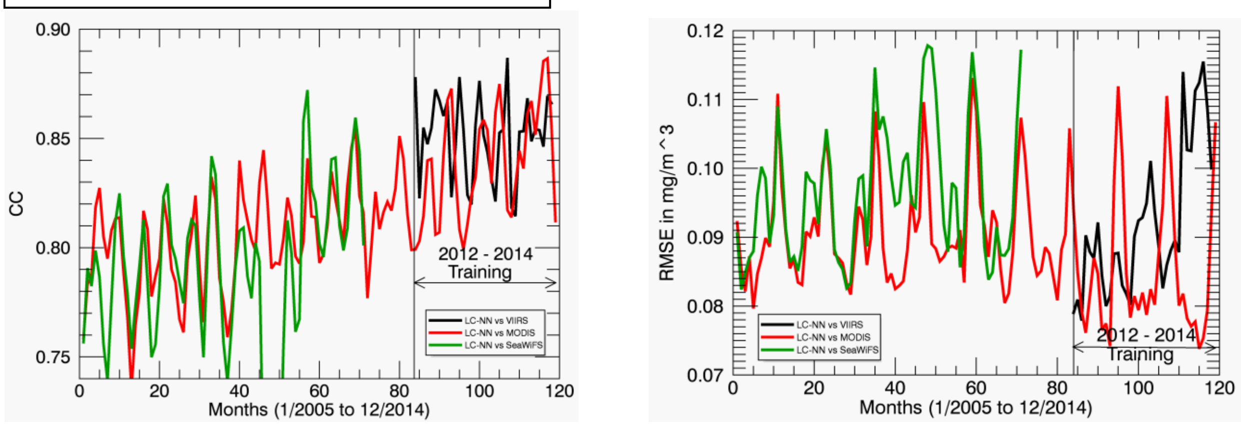

Fig.2 Correlation (left panel) and RMS differences (right panel) between C produced by ensemble of NNs (trained on 3 years of VIIRS data) and C observed by VIIRS (black curves)), MODIS (red curves), and SeaWiFS (green curves).

Assimilating ocean color parameters into ocean models

OC parameters are not prognostic variables in current oceanic models; therefore, OC assimilation requires the coupling of a biochemical component or introducing an observation operator relating C to ocean prognostic variables into the data assimilation system. The NN presented in Eq. (1) can serve as such an operator. The Jacobian of NNs (Eq. 1) can relate innovations in C to innovations in ocean prognostic variables in the data assimilation system [2].

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SMOS Satellite Sea-surface Salinity Data: Impact on Upper-ocean Modelling

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Satellite sea-surface salinity (SSS) observations provide a new means for constraining an important state parameter in numerical ocean models. The benefits of assimilating satellite SSS observations include improved model surface density, near-surface convection, and thermohaline circulation. NOAA's Real-Time Ocean Forecast System (RTOFS)-Global [1] employs an eddy-resolving 1/12th-degree (approximately 9 km horizontal resolution) Hybrid Coordinate Ocean Model (HYCOM) [2]. In the current operational configuration, the RTOFS-Global sea-surface salinity is relaxed to Polar Science Center Hydrographic Climatology version 3.0 (PHC3) SSS fields [3]. Experiments that separately use satellite SSS data and the PHC3 SSS climatology have been conducted to assess the impact of satellite surface salinity measurements on simulated upper-ocean salinity, temperature, and sea-surface height fields.

The first phase of these experiments employs a lower-resolution (1/4th-degree horizontal resolution) HYCOM model. Nine experiments have been performed (Table 1). In the control run, sea-surface salinity is relaxed to an annual cycle of climatological monthly-mean values of SSS (PHC3 climatology). Two sets of cases are then used to explore the model's sensitivity to constraining SSS to satellite measurements, both in terms of relaxation strength and satellite data update interval using monthly-mean and nine-day-mean satellite SSS data from the European Space Agency's Soil Moisture – Ocean Salinity (SMOS) mission [4]. Relaxation strength is modified by changing the e-folding time ($30 \times H_m/H_s$ days), where H_m is the mixed-layer depth and H_s is a reference depth. Greater H_s leads to a shorter e-folding time scale, increasing the constraint on surface salinity by more quickly relaxing surface salinity to the specified SSS reference field.

Table 1. List of experiments

Case	Relaxation Reference SSS	H_s (relaxation strength)
PHC_CL (control)	PHC monthly-mean climatology	15 m
SMOS_MN_15M	SMOS monthly-mean	15 m
SMOS_MN_45M	SMOS monthly-mean	45 m
SMOS_MN_75M	SMOS monthly mean	75 m
SMOS_MN_105M	SMOS monthly mean	105 m
SMOS_9D_15M	9-day mean SMOS	15 m
SMOS_9D_45M	9-day mean SMOS	45 m
SMOS_9D_75M	9-day mean SMOS	75 m
SMOS_9D_105M	9-day mean SMOS	105 m

The results show that the use of satellite SSS data reduces the root-mean-square error (RMSE) of modelled SSS, referenced to SMOS observations (Figs.1a-d). The improvement of SSS is more significant when model SSS is more tightly constrained to observations. On the other hand, increasing data update frequency by using the 9-day-mean SMOS data slightly increases the RMSE of SSS generally everywhere. For the equatorial band 5°S - 5°N, more tightly constraining SSS produces clear and more intense heating along the thermocline in each of the ocean basins (most notably in the Pacific) with the exception of the far western Atlantic, which experiences stronger cooling. The additional signal from increasing the SSS update rate intensifies the monthly-update heating signal along the thermocline, except in the Atlantic, where the additional signal is the opposite of the monthly signal, cooling along most of the thermocline. With more tightly constrained model SSS, salinity is generally fresher everywhere within the 5°S - 5°N equatorial band, except for the eastern Pacific, not including the core of the cold tongue. Intense freshening occurs in the western Pacific, with narrow bands of comparably intense freshening in the Pacific cold tongue and far western Atlantic regions. The freshening seen in the western Atlantic is potentially associated with better representation of freshwater influx from major South American rivers. Increasing the SSS update rate increases salinity relatively uniformly nearly everywhere in the equatorial band, with some narrow intensification in the far eastern and far western portions of each basin. In general, incorporating satellite SSS data improves modeled sea surface height anomalies in the mid-latitude North Atlantic and North Pacific regions.

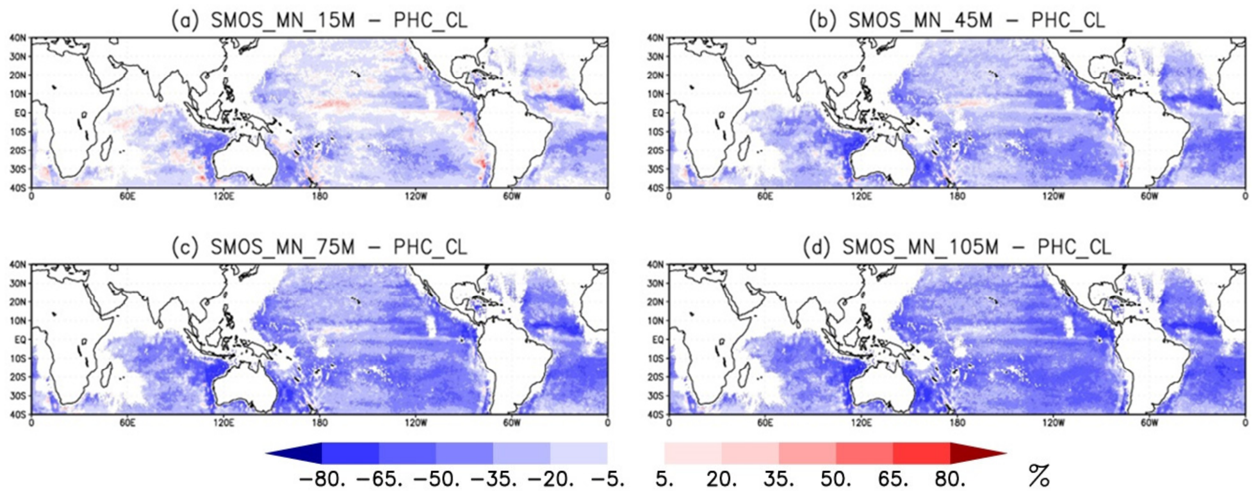

Figure 1. Root mean square error (RMSE) change – SMOS monthly-mean SSS data cases versus control case using PHC SSS climatology, referenced to SMOS observations, with increasing constraint to observed SSS: H_s = a) 15m, b) 45m, c) 75m, and d) 105m.

In terms of constraining models, models have long had a good initial temperature state but not a good initial salinity state. While satellite SSS observations improve the situation, the number of in situ subsurface observations remains inadequate. Modeling needs a mechanism for constraining subsurface salinity values; consequently, research needs to explore not only the use of satellite SSS to constrain modeled surface values but also how to extract/project meaningful values for the upper-ocean.

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Applying Multi-Model Superensemble Methods to Global Ocean Operational Systems

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1. Introduction

A number of international organizations are currently running global Operational Ocean Forecast Systems in near-real-time modes. The daily nowcast and forecast data sets for a variety of oceanographic prognostic parameters are now available to the public through large data servers. Ongoing studies conducted as part of the GODAE OceanView Class-4 intercomparison (Ryan et al., 2015) are demonstrating that these OOS offer complimentary predictive skills. There is also well-documented literature that shows combining multiple forecasts using simple combinations can help to substantially increase accuracy (or reduce error) of such forecasts (Clemen, 1989, Galmarini et al., 2004).

A previous study (Spindler, Mehra, Tolman 2013) employed simple and weighted means and k-means clustering algorithms (Hartigan, 1975; Arthur and Vassilivitski, 2006) to improve nowcast error and bias in SST by processing a month of nowcast fields from five global OOS. This study is an extension of that work into the feasibility of applying simple numerical techniques as well as more sophisticated resampling methods to four global OOS (UKMET GloSea5, US Navy HYCOM, Mercator-Ocean Global, and NCEP Global RTOFS) that offer near-real-time nowcast and forecast data to assess the potential for reducing error and bias in both the current ocean state and forecasts of global SST and North Atlantic potential temperatures to depths of 500 m.

2. Method

Nowcasts and 6 days of forecasts from the member models were processed daily, using 30 prior days of model data to feed into the clustering algorithm. All members were interpolated to the reference data set grid. The global SST ensemble used Nearest Neighbor KD-Tree interpolation, whereas bilinear interpolation both horizontally and vertically was used for the regional ensemble. The external reference field for the global SST was GHRSST at 1/10° resolution, and FNMOC High Resolution Ocean Analysis for GODAE was used for the regional ensemble. Three ensemble methods were compared: simple average, weighted average (using inverse RMSE as the weight), and K-Means cluster-based weighted averaging (which also used inverse RMSE as the weight). Daily RMSE, Bias, and Cross Correlation was computed for both ensembles. For the regional model with depth-dependent fields, vertical temperature profiles were extracted and matched against ARGO profiles used in the GODAE Class-4 intermodel comparison project.

3. Results

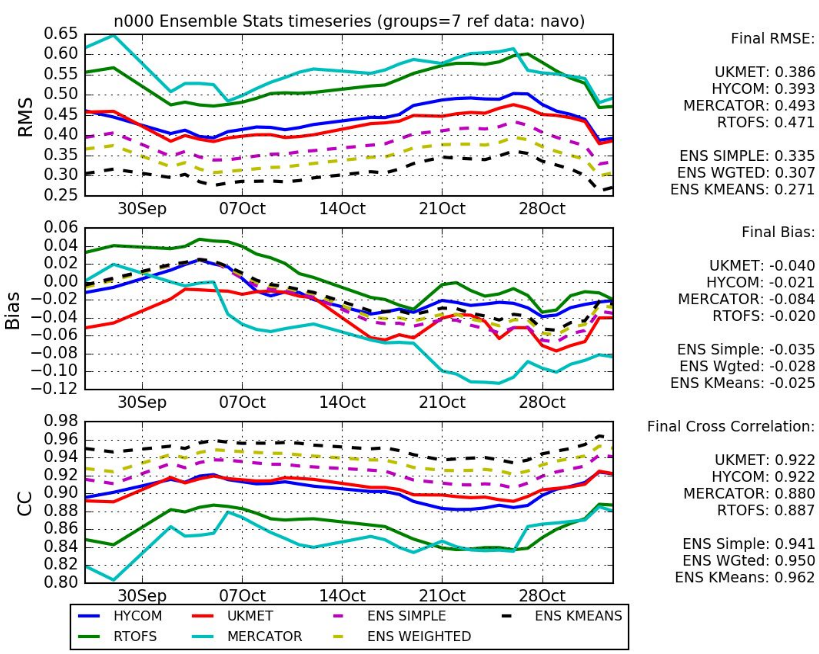

Figure 1. Global SST Ensemble: RMSE, Bias, and Cross Correlation statistics analyzed from one month of model runs. All three methods resulted in reductions in RMSE, improvements in cross-correlations, and with the ensemble bias remaining within the envelope of the members' bias values. The global SST K-Means ensemble exhibited the best improvements, with nowcasts and forecasts showing about a 30% improvement in RMSE, mid-range bias, and about a 10% improvement in the cross-correlation.

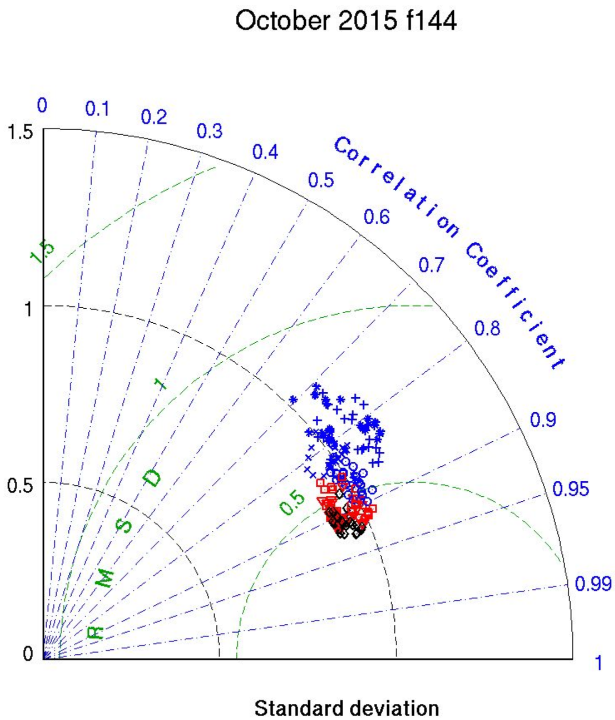

Figure 2: Global SST Ensemble: Taylor Diagram of the model members and ensemble methods for the 144 hour forecasts for the month of October, 2015. All points have been normalized by the standard deviation of the observations.

Blue: Model members
Red: simple and weighted ensemble
Black: K-Means ensemble

The diagram shows significant reductions in the spread of the ensemble RMSE as well as improved cross-correlations of the ensemble forecast as compared to the individual member forecasts. Of the three ensemble methods, the K-Means ensemble shows the lowest RMSE spread and the highest cross-correlation. The model member forecast spread in RMSE was found to increase over the forecast period at a faster rate than the ensemble RMSE spread.

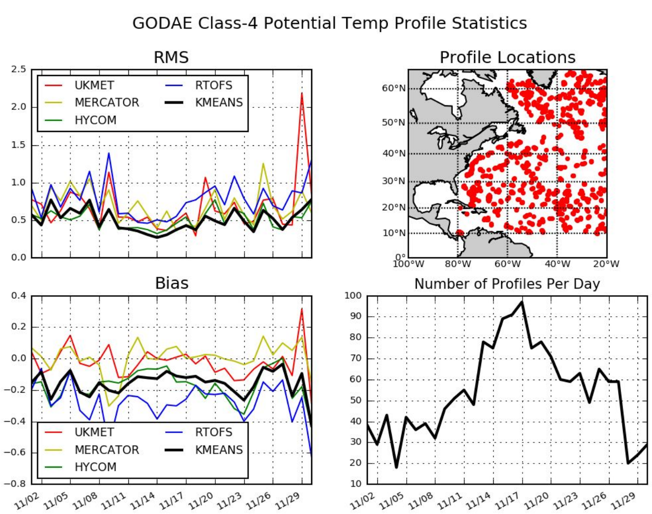

Figure 3: Regional North Atlantic Ensemble: GODAE Class-3 ARGO temperature profiles are compared to co-located profiles extracted from the Regional Ensemble. The upper right panel shows the locations of all of the profiles, the lower right panel shows the number of profiles per day over the course of the month. RMSE of the ensemble profiles showed improvement, but remained just within the envelope of the member values.

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