Supplementary Material

1 Description on the ocean prediction systems used for the observing system evaluation in Section 3

Here, we present the description of the four ocean prediction (data assimilation) systems whose OSE outputs are used for the observing system evaluation in Section 3.

1.1 FOAM

Forecasting Ocean Assimilation Model (FOAM) is the UK Met Office's (UKMO's) analysis and forecast system (Barbosa Aguiar et al., 2024). FOAM is forced by atmospheric forcing from the Met Office NWP system and produces daily analyses and 7-day forecasts. The GOSI9 version of FOAM is used in this study (Carneiro et al., 2024) which consists of the NEMO 4.0.4 ocean model (Guiavarc'h et al., 2024), the coupled SI3 sea ice model (Vancoppenolle et al., 2023) and NEMOVAR data assimilation (Mogensen et al., 2009). The OSEs are performed using Global FOAM with a horizontal resolution of 1/12˚on a tripolar grid and 75 z-coordinate vertical.

TS profiles from EN4 (ref), along-track SLA (CMEMS, 2023a) from four satellites (AltiKa, Sentinel-3a, -3b, and Jason-3), in situ SST from drifter, ships, and buoys, level-2 and level-3 satellite SST data (GCOMW1/AMSR2, JPSS/VIIRS, METOP/AVHRR, MSG/SEVIRI, NOAA/AVHRR, Sentinel-3/SLSTR) and satellite sea ice concentration observations from SSMI/S are also assimilated in FOAM using a 1-day assimilation window. The assimilation method, NEMOVAR, is a multivariate incremental First Guess as Appropriate Time (FGAT) 3DVAR assimilation scheme developed specifically for NEMO (Waters et al., 2015). Variational observation bias correction is carried out for satellite SST using the scheme described in (While and Martin, 2023) and for SLA using the scheme described by (Lea et al., 2008). When assimilating altimeter SLA, it is necessary to add a MDT to the observed SLA to produce an SSH relative to the geoid which can then be compared to the model SSH. The MDT used in the FOAM OSEs is the CNES-CLS13 MDT (Rio et al., 2014). The MDT can have large errors and these are corrected through the variational SLA bias correction scheme. In addition, we have a second variational SLA bias correction which aims to correct for discrepancies in high frequency processes between the model and observation at high latitudes associated with DAC processing in the altimetry observations (Barbosa Aguiar., 2024). BGE covariances in NEMOVAR are specified by defining a field of background error standard deviations and background error correlations for each control vector variable. These are specified through a combination of climatological estimates and flow dependent parameterizations. Multivariate correlations are incorporated in the BGE covariances through linearized balance relationships (Weaver et al., 2005). Water mass conservation properties are used for salinity balance, hydrostatic balance is used for SSH balance and geostrophic balance is used for velocity balance. The assimilation increments are applied to the model using a 24-hour incremental analysis update (IAU) cycle (Bloom et al., 1996).

1.2 GIOPS

The Global Ice Ocean Prediction System (GIOPS) is Environment and Climate Change Canada's (ECCC's) global analysis system (Smith et al., 2016; updated Smith et al., 2024). The analysis system provides initial conditions for several coupled global systems: 10-day deterministic forecasts through the Global Deterministic Forecast System (GDPS; Smith et al., 2018; updated Aider et al., 2024), 16 and 39-day ensemble forecasts through the Global Ensemble Prediction System (GEPS; Peterson et al., 2022; updated Deng et al., 2024), and seasonal forecasts up to 6 months through the Canadian Seasonal and Interannual Prediction System (CanSIPS; Lin et al., 2020). The ocean analysis uses a version of the Système d'Assimilation Mercator version 2 (SAM2) reduced order Kalman Filter assimilation system employed by Mercator Ocean International (Lellouche et al., 2013) described in Smith et al. (2016). Model background and final IAU ocean states are integrated within a NEMOv3.6/CICE6.0 ocean sea ice modeling system (Madec et al., 2008, Hunke et al., 2018) forced by atmospheric fields provided from the IAU stage of the 4DEnVar atmospheric analysis providing the initial atmospheric state for the GDPS system (Buehner, 2015). The ocean model uses an ORCA025 (~1/4°) tripolar grid with 50 levels, identical to the forward forecasting configurations used in the GDPS and GEPS coupled forecasts mentioned above.

The system assimilates TS profiles from CMEMS, along track satellite altimeter observations from 5 satellites (AltiKa, CryoSat, Sentinel-3a, -3b, and Jason-3 [until April 2022]), along with a gridded L4 Optimal Interpolation SST analysis (Brasnett and Colan, 2016) treated as SST observations. This gridded SST analysis is also used as lower boundary conditions for the GDPS atmospheric analysis, so in effort to avoid initialization shock, the surface state of the ocean analysis is constrained tightly (observational error of 0.3°C) to this SST analysis. Assimilation of sea level anomalies from altimeter observations requires the addition of an MDT. The MDT used in GIOPS was updated in the most recent upgrade (Smith et al., 2024) to a hybrid Mercator product described in Lellouche et al (2018) combining the CNES-CLS13 MDT (Rio et al., 2014) with mean innovations of temperature and salinity profiles taken from a multi-decadal ocean reanalysis. The MDT is further iteratively adjusted based on the average SLA innovations from two repeated four-year GIOPS reanalyses produced over the period 2016- 2020 and smoothed using a Shapiro filter to roughly 5° resolution. In addition to the reduced order Kalman filter data assimilation, a 3DVAR large scale bias correction scheme is used whereby TS innovations over the previous four weeks are employed (Lellouche et al., 2013). Error modes (~256) for the assimilation come from an externally forced free run of the ocean model over the period 2001-2011 using daily anomalies with respect to the 30-day running mean. Additionally, a 3DVAR sea ice concentration analysis (Buehner et al., 2016) is blended into the ocean analysis during the IAU phase via the rescaled forecast tendency technique of Smith et al.(2016) to place concentration within the 10 ice thickness categories used in the CICE6 sea ice model.

1.3 MOVE-G3

MOVE/MRI.COM-G3 (MOVE-G3) is a 4DVAR global ocean data assimilation system used as a component of the Coupled Prediction System 3, the current operational coupled atmosphere-ocean prediction system for subseasonal-to-seasonal forecasts in Japan Meteorological Agency (JMA) (Hirahara et al., 2023), and providing oceanic initial conditions to the coupled model in the system. MOVE-G3 is composed of the lower-resolution (0.5˚×1˚) model, G3A, and the higher-resolution (0.25˚×0.25˚) model, G3F. Both models use the code sets of the Meteorological Research Institute Community Ocean Model Version 4 (MRI.COM Ver. 4, Tsujino et al., 2017). They have the global domain, use the tripolar grids (Murray, 1996) with the north poles at 64N-80E and 64N-100W and rescaled height coordinate system (Adcroft and Campin, 2004) with 60 levels, and are forced by the atmospheric forcing based on the JRA-3Q Reanalysis (Kosaka et al., 2024).

TS profiles in the World Ocean Database (Boyer et al., 2016; Locarnini et al., 2013; Zweng et al., 2013), along-track SLA data (CMEMS, 2023a), and SST data drawn from Merged satellite and in situ Global Daily Sea Surface Temperature (MGDSST), produced by JMA (Kurihara et al., 2006), are assimilated into G3A through a 4DVAR scheme with 5-day observation windows, which are performed for every 5 days, and the data-assimilated TS fields are downscaled into G3F through IAU (Bloom et al., 1996). Inadvertently, only the SLA data of two satellites (AltiKa and Cryosat-2) are assimilated in the OSEs, and we plan to re-run the OSEs later with all available SLA data. In the 4DVAR scheme, Vertical coupled TS empirical orthogonal function modes estimated from historical TS observation profiles are used for the BGE statistics, and the satellite SLA data are assimilated by including the term of the misfit of the model SLA to the data in the cost function (Fujii and Kamachi, 2003). The model SLA is calculated from the surface dynamic height (SDH, relative to 2000 m depth) and the MDT estimated from historical TS profiles. The correction of SLA due to the global water mass change is estimated in the 4DVAR. An online bias update scheme (Balmaseda et al., 2007) is applied to TS fields in G3A. Satellite sea ice concentration data estimated from SSMI/S and AMSR2 (Matsumoto et al., 2006) are also assimilated to both G3A and G3F through a separated 3DVAR scheme (Toyoda et al., 2016). You can find the detailed description on MOVE-G3 in Fujii et al. (2023).

1.4 JCOPE-FGO

The Japan Coastal Ocean Predictability Experiments-Forecasting Global Ocean (JCOPE-FGO) is a semi-global ocean nowcasting and forecasting system developed and maintained at Japan Agency for Marine-Earth Science and Technology (JAMSTEC) (Kido et al., 2022; 2023). The OGCM used in JCOPE-FGO is the third-generation model of JCOPE (JCOPE-T; Varlamov and Miyazawa, 2021), and it covers the global ocean from 75°S to 75°N with a horizontal resolution of 0.1°×0.1° and has 44 vertical sigma layers. The model is forced by hourly atmospheric forcing taken the National Centers for Environmental Prediction Climate Forecast System (NCEP CFS, Saha et al., 2010; 2014) as well as the daily river discharge obtained from the JRA55-do dataset (Suzuki et al., 2018; Tsujino et al., 2018).

The first guess values of the model-forecasted TS fields are corrected by analysis values estimated by a 3DVAR scheme (Miyazawa et al., 2009) using the IAU scheme with the assimilation cycle of 7 days. In-situ and satellite data are assimilated into the JCOPE-FGO are same as MOVE-G3; in-situ TS profiles are taken from World Ocean Database, SLAs are drawn from the CMEMS along-track data combining four different satellite altimeters (Jason-3, Cryosat-2, Altika, and Sentinel-3A), and SST are taken from the MGDSST. Here, the time windows for the SSH and SST satellite data are set to 9 days (from -4 days to +4 days), while the time window for the WOD TS is set to 19 days (from -9 days to +9 days). The satellite SLA data are assimilated by including the term of the misfit of the model SLA estimated from SDH (relative to 1500 m depth) to the data in the cost function, as in MOVE-G3 (Fujii and Kamachi, 2003), with the reference MDT being constructed from the climatological T/S fields. Corrections for SLAs due to the global water mass expansion were not made in the present system. More details can be found in the reference paper by Kido et al. (2022).

2 Description on the diagnostics for the observing system evaluation in Section 3

Here, we describe how to calculate the diagnostics used for the observing system evaluation in Section 3. Let $SSH_m(x, y, t, i, j)$ be the output of SSH at location (x, y) and time t from the i-th OSE of the j-th system, with its global mean value removed. Then, the diagnostics for SSH are defined as follows:

RMSD of daily SSH of j-th OSE from ist annual mean (σ_{SSH}):

$$\sigma_{SSH}(x,y,i,j) = \sqrt{\sum_{t=1}^{t_n}\left\{SSH_m(x,y,t,i,j) - \sum_{t'=1}^{t_n} SSH_m(x,y,t',i,j)\right\}^2}.$$

RMSD of daily SSH between the i_1-th and i_2-th OSEs ($RMSD_{SSH}$):

$$RMSD_{SSH}(x,y,i_1,i_2,j) = \sqrt{\frac{1}{t_n}\sum_{t=1}^{t_n}\{SSH_m(x,y,t,i_1,j) - SSH_m(x,y,t,i_2,j)\}^2}$$

RMSE of i-th OSE against the CMEMS L4 SSH ($RMSE_{SSH}$):

$$RMSE_{SSH}(x,y,i,j) = \sqrt{\frac{1}{t_n}\sum_{t=1}^{t_n}\{SSH_m(x,y,t,i,j) - SSH_o(x,y,t)\}^2}$$

SSH multi-system ensemble spread ($Spread_{SSH}$):

$$Spread_{SSH}(x,y,t,i) = \sqrt{\frac{1}{N_s}\sum_{j=1}^{N_s}\left\{SSH_m(x,y,t,i,j) - \frac{1}{N_s}\sum_{j'=1}^{N_s} SSH_m(x,y,t,i,j')\right\}^2}$$

Here, t_n is the number of the days in the analyzed year, 2020, N_s is the number of the system whose outputs are available, and SSH_o is the CMEMS L4 SSH from altimetry objective analysis (CMEMS, 2023b), with its global mean removed. The mean difference between the SSH model outputs and CMEMS SSH, that is the bias, is not removed when calculating the RMSEs. The global mean is removed from both the OSE SSH outputs and L4 SLA because ocean models in most prediction systems adopt the Boussinesq approximation and hence do not usually represent the variation of the global mean SSH associated with thermal expansion of seawater and global fresh water mass change.

Likewise, the RMSEs of TS against observed values of the reference Argo floats ($RMSE_T$ and $RMSE_S$) are calculated as follows:

$$RMSE_T(z) = \sqrt{\frac{1}{N}\sum_{l=1}^{N}\{T_m(z,l) - T_o(z,l)\}^2},\quad RMSE_S(z) = \sqrt{\frac{1}{N}\sum_{l=1}^{N}\{S_m(z,l) - S_o(z,l)\}^2},$$

where T_m and S_m are the TS outputs from OSE at the position of the reference Argo profile, T_o and S_o are the TS values observed by the reference Argo floats, and N is the number of the reference Argo profiles in the target region. The TS observations of the reference Argo floats are collected from the snapshot of the Argo GDAC in Oct. 2023. Only the data to which delayed mode quality control is applied and where the maximum depth with valid temperature values exceeds 100 m are used as the reference here. The mean difference between the TS outputs and observed values (i.e., the bias), is not removed when calculating the RMSEs.

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