A balanced Kalman Filter ocean data assimilation system with application to the South Australian Sea

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Abstract

In this paper, an Ensemble Kalman Filter (EnKF) based regional ocean data assimilation system has been developed and applied to the South Australian Sea. This system consists of the data assimilation algorithm provided by the NCAR Data Assimilation Research Testbed (DART) and the Regional Ocean Modelling System (ROMS). We describe the first implementation of the physical balance operator (temperature-salinity, hydrostatic and geostrophic balance) to DART, to reduce the spurious waves which may be introduced during the data assimilation process. The effect of the balance operator is validated in both an idealised shallow water model and the ROMS model real case study. In the shallow water model, the geostrophic balance operator eliminates spurious ageostrophic waves and produces a better sea surface height (SSH) and velocity analysis and forecast. Its impact increases as the sea surface height and wind stress increase. In the real case, satellite-observed sea surface temperature (SST) and SSH are assimilated in the South Australian Sea with 50 ensembles using the Ensemble Adjustment Kalman Filter (EAKF). Assimilating SSH and SST enhances the estimation of SSH and SST in the entire domain, respectively. Assimilation with the balance operator produces a more realistic simulation of surface currents and subsurface temperature profile. The best improvement is obtained when only SSH is assimilated with the balance operator. A case study with a storm suggests that the benefit of the balance operator is of particular importance under high wind stress conditions. Implementing the balance operator could be a general benefit to ocean data assimilation systems.

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1. Introduction

By using the Bayesian theorem, data assimilation provides an objective criterion for fusing observations with numerical models to produce an estimate of the true state (e.g. Lahoz and Schneider, 2014; Wikle and Berliner, 2007). This is a crucial step in providing an optimal initial condition for ocean forecasting (e.g. Lahoz and Schneider, 2014; Blayo et al., 2014). Global ocean data assimilation has developed rapidly during the past decade, and an increasing number of products are provided by groups worldwide (e.g., Global Ocean Data Assimilation Experiment, <https://www.godae-oceanview.org/>). However, the typical resolution of global models is still too low to resolve mesoscale features thus there is a need to develop regional ocean data assimilation systems (Moore et al., 2013).

There are two popular data assimilation approaches: variational and sequential (Lahoz and Schneider, 2014). The variational approach adjusts the model trajectories to fit the observations by minimising the cost function. On the other hand, the sequential approach updates the model state by comparing the mean and variability of both model and data, each time when the new observation is available. These two approaches are both based on the Bayesian theorem and can be simplified to similar algorithms under the assumptions of Gaussianity and linearity. The detailed description of data assimilation algorithms has been explored extensively (e.g. Lahoz and Schneider, 2014; Wikle and Berliner, 2007; Evensen, 2009).

The Kalman Filter (Kalman, 1960) is a sequential data assimilation algorithm designed for a linear dynamical model with Gaussian-distributed model and observation errors. Evensen (1994) developed the ensemble method by using a Monte Carlo technique to approximate the mean and covariance of a high-dimensional system. Compared with the variational data assimilation such as four-dimensional variational method (4DVAR), EnKF needs much less effort to implement since the tangent linear and adjoint models are not needed. It is also possible to use different physical schemes in the ensemble members.

EnKF has been used in several regional ocean data assimilation studies. Evensen and van Leeuwen (1996) developed the first EnKF based regional

data assimilation system for the Agulhas current using a quasigeostrophic model. Seo et al. (2010) assimilated SST in a northwest Pacific ROMS model through a stochastic EnKF scheme, but only SST was assimilated and physical balance was not studied. Here we present the first implementation of DART (Anderson et al., 2009), a community data assimilation facility to ROMS, to provide several state-of-the-art algorithms with localisation, inflation techniques. Also, we use balance constraints to reduce the spurious waves generated in the data assimilation process.

The localisation technique is needed to reduce the harm caused by the spurious covariances with distant grid points in EnKF with limited ensemble members (Lorenc, 2003; Houtekamer and Mitchell, 2001; Gaspari and Cohn, 1999). However, localisation may cause imbalance to the dynamical system (Lorenc, 2003; Greybush et al., 2011), although a balanced model error covariance produces balanced analysis state (Cohn and Parrish, 1991). Lorenc (2003) pointed out that when SSH observation at a single point is assimilated without localisation, the increments of SSH and ocean currents are balanced. If localisation is used, the gradient of SSH increases while the ocean currents reduce. Therefore spurious ageostrophic waves are created in this process. A schematic description of this example can be found in Greybush et al. (2011) (in their Fig. 1). Mitchell et al. (2002) reported that different ensemble size, assimilating frequency or localisation radius can cause imbalance for GCMs. Kepert (2009) suggested using localisation of streamfunction and velocity potential instead of u and v velocities, but this method is not easy to implement for regional ocean models. For the multivariate problem, it is also difficult to specify the relationship among various variables. A common practice is to use linear regression, but this can be a major source of error (Anderson, 2007b). To solve this problem, Anderson (2007b) proposed to ‘localise’ the impact of observation to model states (e.g., SST observation at one point and simulated ocean currents at another point), but he also pointed out that it is usually difficult to define the ‘distance’ between them, especially for high-dimensional GCMs. In this paper, we use a multivariate balance operator proposed by Weaver et al. (2005) to solve the imbalance problem. In this algorithm, each model variable is separated into balanced and unbalanced components, and several balance assumptions are made to calculate the increments. This physical constraint has been used in several variational ocean data assimilation systems (e.g. Balmaseda et al., 2013; Li et al., 2008; Moore et al., 2011c).

The DART/ROMS data assimilation system is applied to the South Aus-

tralian Sea (31.5°S to 39.5°S, 117°E to 140°E). This region hosts the world's longest zonal, mid-latitude shelf (about 2500km) between Cape Leeuwin and Portland (Middleton and Bye, 2007). The Leeuwin Current, flowing southward from the tropics near the west coast of Australia, enters the South Australian Sea around Cape Leeuwin and extends to Tasmania. This region is recognised as one of the 64 Large Marine Ecosystems (LMEs) by NOAA (<http://www.lme.noaa.gov/>). There are also emerging tourism ventures and oil/gas exploration. The simulation and prediction of the ocean circulation, temperature and other oceanic variables are therefore necessary.

In this paper, we first describe the data assimilation system and the balance operator in Section 2. In Section 3 we evaluate the effect of balance operator using an idealised two-dimensional shallow water model. The results of the South Australian Sea model are given in Section 4. In Section 5 we discuss and analyse the results from Section 3 and 4. A summary concludes this paper in Section 6.

2. Method and data

The Ensemble Adjustment Kalman Filter (EAKF) (Anderson, 2001) is implemented as the data assimilation algorithm. We introduce a physical balance operator to this system and analyse the performance in both an idealised shallow water model and the ROMS real case.

2.1. Ensemble Kalman Filter and the balance operator

There are many implementations of the ensemble Kalman Filter (e.g. Evensen, 2003; Houtekamer and Mitchell, 2001; Anderson, 2001). The data assimilation cycle consists of two stages. Firstly, in the forecasting stage, the model state x evolves through a dynamic model and secondly in the analysis stage the estimation of model state is improved by comparing the forecast x^f and the observation y^o , the analysis is computed as,

$$x^a = x^f + K[y^o - H(x^f)], \quad (1)$$

where B is the model error covariance matrix, R is the observation error covariance. H is the observation operator that projects the model state x to the observation space $y = H(x)$. The difference between x^a and x^f is defined as the increment Δx . The optimal variance minimising weight is given by the Kalman gain,

$$K = BH^T(HBH^T + R)^{-1}, \quad (2)$$

104 In the ensemble data assimilation approach, the B matrix is computed
105 from the N ensemble members in each data assimilation cycle as,

$$B = X^f X^{fT}, \quad (3)$$

106 where $X = \frac{1}{\sqrt{N-1}}(x_1 - \bar{x}, x_2 - \bar{x}, \dots, x_N - \bar{x})$ is the perturbation matrix whose
107 columns are the deviations from the ensemble mean.

108 For an ocean model such as ROMS, there are 5 components in the state
109 vector x : sea surface height η ; potential temperature T ; salinity S ; horizontal
110 velocities u and v . Temperature is usually the most observed variable in the
111 ocean so Weaver et al. (2005) proposed to compute the relations between
112 the variables based on T . Each variable except T is decomposed into two
113 components, the balanced component and the unbalanced one. Therefore
114 the perturbations δx can also be decomposed as following,

$$\begin{pmatrix} T \\ S \\ \eta \\ u \\ v \end{pmatrix} = \begin{pmatrix} T \\ S_B \\ \eta_B \\ u_B \\ v_B \end{pmatrix} + \begin{pmatrix} 0 \\ S_U \\ \eta_U \\ u_U \\ v_U \end{pmatrix} = L \begin{pmatrix} T \\ S_U \\ \eta_U \\ u_U \\ v_U \end{pmatrix}, \quad (4)$$

115 where the variables with subscript B represent the balanced component of
116 the variables while those with subscript U represent the unbalanced one. The
117 balanced part of variable x_1 can be derived from other variable x_2 through
118 the linear balance operator L . The details of L are explained in Appendix
119 A.

120 The model error covariance is thus converted to,

$$B = LB_u L^T, \quad (5)$$

121 and Eq.1 is written as,

$$x^a = x^f + LB_u L^T H^T (H LB_u L^T H^T + R)^{-1} [y^o - H(x^f)], \quad (6)$$

122 where B_u is the error covariance of the unbalanced components. Here we
123 assume that the balanced components of the ocean state are correlated while
124 the unbalanced residuals are uncorrelated (Weaver et al., 2005).

125 An update scheme is designed based on this algorithm. This scheme starts
 126 from an ensemble of initial model states or short-term forecast, then the
 127 balanced component is calculated and the unbalanced component is derived.
 128 B_u is computed from the unbalanced component, after which the model states
 129 are updated using Eq.6 (Fig. 1).

130 2.2. Shallow water model

131 The prediction of ocean currents is of particular interest and satellite
 132 observed SSH is the most widely used variable in data assimilation systems
 133 to constrain the ocean currents (e.g. Jacobs et al., 2014). It is necessary
 134 to validate the effect of the geostrophic balance operator on ocean currents.
 135 Here we use a two-dimensional shallow water model to initially evaluate
 136 the effect of the balance operator. The shallow water equations describe a
 137 rotating (with constant Coriolis parameter), inviscid fluid with wind forcing
 138 in the x direction. Similar shallow water models have been used to study
 139 the physical balance (e.g. Kepert, 2009; Greybush et al., 2011). The model
 140 equations are,

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - f v + \tau &= -g \frac{\partial \eta}{\partial x} \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + f u &= -g \frac{\partial \eta}{\partial y} \\ \frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x}[u(h + \eta)] + \frac{\partial}{\partial y}[v(h + \eta)] &= 0 \end{aligned} \quad , \quad (7)$$

141 where η is the free surface displacement, h is the bottom topography (50 m in
 142 this experiment), τ is the wind forcing, and f is the Coriolis parameter. We
 143 set the Coriolis parameter to 10^{-4}s^{-1} , a typical value for the mid-latitude.
 144 The model is constructed on a 2000 by 2000 km domain with 10 km hori-
 145 zontal resolution in both x and y direction and forced by periodic boundary
 146 conditions.

147 Each ensemble is initialised from meridional η ridges,

$$\eta(x) = \eta_0 \cos\left(\frac{2\pi}{L}(x - x_{ps})\right), \quad (8)$$

148 where L is the wavelength and in the true state L is set to 200 km, η_0 is
 149 the amplitude and x_{ps} is the wave phase shift. Each ensemble is forced by a
 150 periodic zonal wind stress τ with a period of 48 hours,

$$\tau(t) = \tau_0 \cos\left(\frac{2\pi}{t_\tau}(t - t_{ps})\right), \quad (9)$$

151 where τ_0 is the amplitude, t_τ is the period (48 hours), and t_{ps} is the wave
 152 phase shift. The initial sea surface height of each ensemble member is gener-
 153 ated by shifting the phase of the true initial state x_{ps} by a uniform random
 154 distribution of $[20, 40]$ km and the amplitude η_0 by $[-0.05, 0.05]$ m. In the
 155 initial condition of the true state and each ensemble member, the velocities
 156 are calculated according to the geostrophic balance. The wind forcing of
 157 each ensemble member is perturbed by randomly shifting the amplitude by
 158 $[-10\%, 10\%]$ and the phase by $[-3, 3]$ hr. A schematic setup of the model is
 159 displayed in Fig. 2.

160 We first integrate the true state through a Lax-Wendroff scheme, with a
 161 time step 6 s, for 576000 steps, or 40 days. The observations of η are then
 162 created by adding a Gaussian distributed white noise with 0 m mean and 0.03
 163 m standard deviation to the true state. The locations of the observations are
 164 selected along 4 diagonal tracks with a 10km interval to mimic the satellite
 165 tracks. The period of the observations is set to 24 hours, and the observation
 166 tracks move eastward at a 3000 km/day speed similar as the real satellite
 167 tracks. We conduct two sets of experiments by varying the initial SSH and
 168 wind stress, as described in Table. 1. In both the shallow water case and
 169 the ROMS real case, a background covariance matrix localisation technique
 170 (Gaspari and Cohn, 1999) is used. Two localisation scales (60 km and 100
 171 km, the scale is the halfwidth of the Gaspari Cohn parameter in this paper,
 172 as the default setup in DART) are used in the idealised case. Larger scales
 173 have been tested but the resulting SSH and velocity fields are over-smoothed
 174 and thus not used here. In each experiment, the ensemble size is set to
 175 100 and the error of the observations is set to 0.03 m. Each experiment is
 176 integrated for 40 days by assimilating sea surface height only with a 24-hour
 177 assimilation window and the results of the last 30 days are analysed.

178 *2.3. Application of the ROMS/DART system in the South Australian Sea*

179 *2.3.1. Configuration of DART*

180 DART is ‘an open-source community facility that provides software tools
 181 for data assimilation research, development, and education’ (Anderson et al.,
 182 2009) developed and maintained by the Data Assimilation Research Section
 183 (DARes) at the National Center for Atmospheric Research (NCAR). DART
 184 provides several deterministic and stochastic algorithms, including Ensemble

185 Adjustment Kalman, Ensemble Kalman, Kernel and Particle filters. These
186 algorithms have been used in different atmosphere and ocean general cir-
187 culation models (Anderson et al., 2009) including both regional (MITgcm)
188 (Hoteit et al., 2013) and global (POP) (Karspeck et al., 2013) ocean models.

189 One of the major problems facing the traditional EnKF is that the en-
190 semble size is usually too small to calculate the statistics. In this paper, a
191 deterministic algorithm, the Ensemble Adjustment Kalman Filter (EAKF)
192 (Anderson, 2001, 2003) is used. EAKF is a type of ensemble square root fil-
193 ter (Tippett et al., 2003) and in this algorithm the model state is computed
194 through an adjustment matrix so that the posterior covariance satisfies the
195 Kalman gain exactly.

196 Assimilation of each observation adds information to the dynamic system
197 and thus the spread of the ensemble decreases. This reduction of ensemble
198 spread could be problematic due to the model and observation error and bias.
199 The problem is addressed in DART by inflating the spread periodically. The
200 inflation must vary spatially and temporally to improve analysis and fore-
201 cast. DART employs a hierarchical Bayesian filter (HBF) adaptive inflation
202 algorithm (Anderson, 2007a) to produce varying inflation. If the observation
203 is further from the ensemble mean than expected, HBF uses more inflation
204 and vice versa. In the ROMS case, only prior inflation is used and the infla-
205 tion is assigned with initial value of 1.02, the lowerbound of 1.0, the inflation
206 damping of 0.9 and evolves with the standard deviation of 0.6. In most of the
207 experiments, the actual inflation coefficient is 1 to 6, which is a reasonable
208 value. In the idealised shallow water model, no inflation is used.

209 Another challenge for ensemble methods with small ensemble size is the
210 spurious long-distance correlations (Houtekamer and Mitchell, 1998). The
211 localisation technique is usually used to suppress the influence of distant ob-
212 servations (e.g. Mitchell et al., 2002). The optimum choice of the localisation
213 scale depends on several factors such as the ensemble size (e.g. Mitchell et al.,
214 2002) and sampling correlation (e.g. Emerick and Reynolds, 2011). The lo-
215 calisation radius halfwidth is set to 0.03 arc in the ROMS case, which is
216 about 110 km in the region. This value is selected after comparing a series of
217 assimilation experiments (not shown here) with different localisation config-
218 urations (0.02 arc, 0.03 arc, 0.04 arc and 0.05 arc). Generally, a larger scale
219 produces a better result for SSH while a smaller one produces better SST.
220 The results with the scale of 0.03 arc are overall the best for both variables.

221 The initial state ensemble is essential for the success of data assimilation
222 as it provides information about the variability and uncertainty of the system.

223 An appropriate initial ensemble should include ‘information about the main
 224 physical quantities that govern the evolution of the state’ thus it could speed
 225 up convergence toward the ‘true’ ocean state (Hoteit et al., 2008). Following
 226 Hoteit et al. (2013), a second-order sampling scheme (Pham, 2001) is used
 227 to generate the initial ensemble. Firstly, we create a set of model states
 228 using the results of the control run (in this study, a 7 year control run, as
 229 described in the following section) in winter since the South Australian Sea
 230 is dominated by strong seasonality (Middleton and Bye, 2007). Secondly,
 231 an Empirical Orthogonal Function (EOF) analysis is applied to extract the
 232 dominant variability from this long model trajectory. Then the initial states
 233 are generated using the following equation,

$$x_0^i = \bar{x} + \sqrt{N} L_0 \sigma_i^T, \quad (10)$$

234 where N is the ensemble size, L_0 is the matrix whose $N - 1$ columns are
 235 the EOFs, $\bar{x}$ is the mean of the long-term trajectory and σ_i is the i th of a
 236 $(N - 1) \times N$ random matrix with orthonormal columns and zero column sums.
 237 The ensemble size is determined according to the limitation of computation
 238 resource and model variance, in this study the ensemble size is 50. The
 239 ensemble members are thus generated with mean $\bar{x}$ and covariance matrix
 240 $L_0 L_0^T$ which is an optimum approximation of the original states (Hoteit et al.,
 241 2013). The ensemble is then used to initialise DART.

242 *2.3.2. Configuration of ROMS*

243 ROMS is a free-surface, hydrostatic, primitive equations ocean model
 244 with a terrain-following coordinate system (Haidvogel et al., 2008; Shchep-
 245 etkin and McWilliams, 2005, 2009). It has been widely used for a diverse
 246 range of applications (e.g. Haidvogel et al., 2000; White and Toumi, 2014;
 247 Wilkin et al., 2005). In addition, ROMS is one of the few community ocean
 248 models which support 4D-VAR (e.g. Moore et al., 2011a,b,c; Song et al.,
 249 2012).

250 The ROMS model is implemented in the South Australian Sea on a
 251 10 km horizontal grid with 35 vertical layers. The vertical coordinate is
 252 set to a minimum depth of 5 m and a maximum depth of 5000 m. The
 253 4th-order centred vertical advection and 3rd-order upstream horizontal ad-
 254 vection schemes are used for tracer advection. The horizontal advection
 255 of momentum is calculated using a 3rd-order upstream split scheme with
 256 the Smagorinsky-like viscosity applied, and the vertical advection of mo-
 257 mentum is calculated using a splines scheme. The model domain extends

from 39.5°S to 31.5°S and 117°E to 140°E. The bathymetry is obtained from the Scripps Institute of Oceanography global seafloor topography (Smith, 1997). Tidal sea level and horizontal velocity are extracted from Oregon State University TPXO7.2 global inverse tidal model at 1/12° resolution (<http://volkov.oce.orst.edu/tides/global.html>). The initial and lateral boundary conditions for temperature, salinity, three-dimensional velocity fields, and non-tidal sea level are obtained from the daily mean, 1/12° HYCOM re-analysis (Metzger et al., 2014). The model is forced with the 6-hourly re-analysis atmospheric state from the National Centers for Environmental Prediction (NCEP) Climate Forecast System Re-analysis (CFSR) project (Saha et al., 2010). The atmospheric forcing variables include downward longwave radiation, downward shortwave radiation, sea level pressure, 2m specific humidity, 2 m air temperature, 10 m winds, and total precipitation. Climatological river discharge is obtained from RivDIS database (Vorosmarty et al., 1998) provided by KNMI (<http://climexp.knmi.nl/>) to calculate the flow rate of the major river (River Murray) in this region.

2.3.3. Experiment design

The control simulation runs for 8 years from 2005 to 2012. The first year is discarded as the spin-up period. The data assimilation simulations all run from January 2007 to June 2007. In the data assimilation experiments, the AVISO along-track sea surface height (SSH) anomalies (<http://www.aviso.altimetry.fr/en/home.html>) and TMI along-track sea surface temperature (SST) dataset (<http://www.remss.com/missions/tmi>) are assimilated every five days. Here all observations within ± 2.5 days of the assimilation time are binned as if they were available at the middle of this assimilation window. This window length is similar with previous studies (e.g. Hoteit et al., 2013; Oke et al., 2013). The main variability from the 30 year CFSR data for each month are extracted using EOF analysis and the atmospheric forcing for each of the ensemble members is created in a similar way as the initial ensembles,

$$x^i = x + 0.2 * \sqrt{N} L \sigma_i^T, \quad (11)$$

where x is the forcing variables (wind field and radiation in this paper), L is the EOF matrix of the 30 year (1981-2010) data during the appropriate month of the forcing, and σ_i is the random matrix as described in Eq. 10. Thus the forcing for each ensemble member is different, and the error of

292 CFSR is assumed to be 20%. The open boundary forcing is from HYCOM
293 analysis and unvaried.

294 AVISO merges observations from different satellites but only Jason-1,
295 Geosat and Envisat were operating during our data assimilation period. Fol-
296 lowing Moore et al. (2011a), the AVISO data is processed before being assim-
297 ilated by adding the observed sea level anomalies to the difference between
298 the ROMS mean SSH and AVISO dynamic topography for 2006-2012 to re-
299 move the offset between the model SSH and AVISO dynamic topography.
300 Because the AVISO SSH data is de-tided, we use the FES2012 tidal model
301 (Lyard et al., 2006) to add the tidal signal to the original AVISO SSH. The
302 water levels simulated by ROMS and FES2012 model are similar in most of
303 the domain, but in regions where the ocean is shallow and bathymetry is
304 complicated, they are different. Therefore the data within 100 km distance
305 of the coastline is discarded. TMI (TRMM Microwave Imager) is one of the
306 5 instruments carried by TRMM (the Tropical Rainfall Measuring Mission),
307 which launched on 27 November 1997. TMI measures SST in addition to
308 rainfall, sea surface wind speed, column water vapour and cloud liquid wa-
309 ter. The SST data within 100 km distance to the coastline is considered
310 not reliable (Hoteit et al., 2013) and is discarded. 5 data assimilation ex-
311 periments are carried out to assimilate SST and SSH with/without balance
312 operator. The setup of all experiments is summarised in Table 2.

313 We use both gridded data products and direct observations to evaluate
314 the effect of data assimilation. The comparison with gridded products, in-
315 cluding AVISO $1/4^\circ$ gridded daily dynamic topography, OISST version 2
316 daily SST data and Ocean Surface Current Analysis Real-time (OSCAR;
317 Bonjean and Lagerloef, 2002) currents, illustrates the effects over the whole
318 domain. The AVISO gridded data is processed similarly to the along track
319 data to ensure the spatiotemporal mean of AVISO and model SSH are equal.
320 The OISST data composites observations from different platforms (satellites,
321 ships, buoys) on a $1/4^\circ$ global grid and the gaps are filled by interpolation
322 (Reynolds et al., 2007). The OSCAR data provides $1/3^\circ$ 5-day mean near
323 real-time global ocean currents products of the top 30 m calculated from
324 satellite altimetry and wind fields. Although the more complex physical pro-
325 cess is missing, OSCAR provides ‘as close to a direct satellite measurement of
326 surface currents on a fixed global grid at regular intervals as possible’ (Dohan
327 and Maximenko, 2010). Ocean surface currents from 7 drifters (2791 data
328 points) (http://www.aoml.noaa.gov/phod/dac/gdp_drifter.php; Lump-
329 kin and Pazos, 2007) and subsurface temperature and salinity observed by

330 8 Argo floats (198 profiles) are also used to provide independent validation.
 331 The ARGO floats were located around 120°E, 25.5°S and the drifters were
 332 distributed in the south part of the domain (Fig. 5).

333 3. Results

334 3.1. Shallow water model

335 Lorenc (2003) pointed out that assimilating SSH in a shallow water model
 336 creates spurious ageostrophic waves. Fig. 3 shows the increments at the 25th
 337 data assimilation cycle with 0.2 Pa wind stress and 100 km localisation ra-
 338 dius. The increment in the unbalanced experiment is strongly ageostrophic
 339 (Fig. 3(B)) while in the balanced experiment there is no ageostrophic cur-
 340 rent increment. The localisation reduces both SSH and velocities proportion-
 341 ally but increases the SSH gradient. In addition, the wind forcing creates
 342 ageostrophic currents in the prior state and, in the unbalanced experiment,
 343 this signal propagates to the increment through the multivariate regression.
 344 Therefore, a spurious ageostrophic shock is created in the posterior state and
 345 this affects the performance of data assimilation. Theoretically, the dynami-
 346 cal model is able to adjust and restore to a balanced state even it starts with
 347 spurious waves. However, this restored state is different from the one starting
 348 from a balanced state (not shown). In addition, this geostrophic adjustment
 349 in the dynamical model is usually not fast enough. The ageostrophic cur-
 350 rents in the 24 hour forecast is stronger by around 3 cm/s in the unbalanced
 351 experiment than in the balanced experiment, when the wind stress is 0.2 Pa.
 352 Thus the balance operator is needed to reduce the misfit between the truth
 353 and assimilations in different scenarios.

354 The balance operator reduces the error of different variables in varying
 355 wind forcing and initial SSH displacement scenarios. Here we use the Root
 356 Mean Square Error (RMSE) between the simulation and the true state as the
 357 metric for evaluating the assimilation. Fig. 4(a) and (b) display the RMSE
 358 of SSH and v velocity as a function of initial η amplitude (the amplitude
 359 does not change much in the integration), respectively. It is evident that
 360 the data assimilation with the balance operator produces a lower error for
 361 both sea surface height and velocity estimation compared to the unbalanced
 362 approach. Although the RMSE increases as the amplitude increases, the rel-
 363 ative advantage of the balance operator also increases. In addition, a longer
 364 localisation radius is better than a shorter one for either method. However,

the balanced method with smaller localisation radius outperforms the original method with the larger radius. When both use a larger radius (100 km), the balanced data assimilation produces a 17% lower average RMSE than the unbalanced approach (5.2 cm and 6.2 cm respectively) for the SSH and 11% for the v velocity (16 cm/s and 18 cm/s respectively).

When forced by varying wind stress, the balance operator also improves the data assimilation performance although the error in both experiments is higher than that with fixed wind forcing, because of the noisy forcing (Fig. 4(c) and (d)). With a 100 km localisation radius, the average error of SSH decreases 12% from 4.2 to 3.7cm and the error of v reduces 9% from 22cm/s to 20cm/s. In the ocean, the typical value of SSH is around 10 to 20 cm while the wind stress is around 0.1 Pa. In those conditions, the balance operator reduces the RMSE of SSH and velocity by 12% (from 2.3cm to 2.0cm) and 7% (from 13cm/s to 12cm/s), respectively. The effect of the balance operator is more significant when the wind stress is larger. This is because the ageostrophic component in the prior ensembles increases as the wind stress increases, thus the increments of ageostrophic current in the unbalanced experiment get stronger. For example, when the wind stress is as large as 0.3 Pa the error increases significantly and the advantage of the balance operator is 17% and 11% for η and v respectively.

3.2. The South Australian Sea case

3.2.1. Control run

Before conducting data assimilation for the real case, a model capable of producing reasonable climatology is required. Fig. 5 displays the comparison between the simulated SST and the OISST dataset. Both the mean and the variability of the model results and observation are in good agreement. The model reproduces the warm pattern with little variability along the coast, which is a main feature of the north boundary currents. The model also captures the high variability in the shallow water region of the Spencer Gulf and the Gulf St Vincent. However, the model variability in the central western part is greater than OISST, which indicates a stronger meandering of the north boundary currents than observed.

An EOF analysis is carried out to extract the main variability of SLA. The first 2 EOFs of the original SLA (not shown) in ROMS and AVISO are similar. They represent the seasonal cycle and explain 70% - 80% of the variability. Fig. 6 depicts the first 2 EOFs of the deseasonalised SLA from ROMS and AVISO. The first EOF represents an annual cycle overlapped

402 on a low-frequency oscillation near the coastline. ROMS shows a similar
 403 spatiotemporal pattern with AVISO. The second EOF of AVISO represents
 404 high-frequency eddy events in the west of the domain while for ROMS there is
 405 a larger feature in the middle of the domain. The model reproduces the sea-
 406 sonal cycle and low-frequency feature, but the eddy activity is not captured
 407 well.

408 In the 7 year mean of simulated surface currents, the strong eastward
 409 north boundary currents in winter and weak westward currents in the summer
 410 are also reproduced (not shown), as seen in the observed climatology (e.g.
 411 Middleton and Bye, 2007, in their Fig. 2).

412 3.2.2. Standard data assimilation

413 SST and SSH are assimilated in these experiments, together and sepa-
 414 rately. The results suggest that assimilating SST and SSH improves these
 415 two variables, and assimilating SSH also produces a better subsurface tem-
 416 perature profile. However, unlike in some other studies (e.g. Hoteit et al.,
 417 2013; Kurapov et al., 2011), SSH assimilation does not generate a more ac-
 418 curate SST distribution. When both SST and SSH are assimilated at the
 419 same time, the correction to both SST and SSH field is very similar to that
 420 of the SST assimilation only. We validate the performance of data assimi-
 421 lation by comparing the domain-averaged RMSE of SST and SSH for different
 422 experiments. The error of surface and subsurface temperature is calculated
 423 against the OISST dataset and Argo observations. Compared to the control
 424 run (ExpA), assimilating SST alone (ExpC) reduces the SST error by 58%
 425 from 0.86°C to 0.36°C (Fig. 7(A) and Table 3), and the error decreases from
 426 above 0.7°C in most of the domain to around 0.3°C . The 5-day forecast is
 427 also much better ($\text{RMSE} = 0.55^{\circ}\text{C}$) than the control run (Fig. 7(B)). The
 428 difference of RMSE between assimilating SST with (ExpD) and without SSH
 429 is marginal (RMSE for posterior state is 0.37°C), indicating that the process
 430 of SST adjustment is mainly determined by the assimilation of SST. The
 431 SST observations are more numerous ($\sim 3200/\text{day}$) and have a bigger spatial
 432 coverage than the SSH observations ($\sim 400/\text{day}$). In addition, the error of
 433 SST mainly provides information about the surface heat flux which has lit-
 434 tle effect on SSH. A finer tuning of SSH/SST combination may improve the
 435 results. On the other hand, when assimilating SSH (ExpB), the RMSE is
 436 quite similar to the control run and the spatial pattern is also similar. The
 437 comparison with Argo temperature and salinity profiles (Fig. 8, Table 3)
 438 shows that, although the subsurface variables are not assimilated, a better

distribution is reproduced. For instance, assimilating SSH alone reduces the RMSE of temperature and salinity by 12% (0.14°C) and 10% (0.02 PSU), respectively, in the upper 300 m. In ExpC (assimilating SST alone), the error of temperature reduces by 10% (0.12°C) in the upper 300 m but increases by 7% (0.07°C) in 300-700 m, indicating the simulation of ocean circulation is degenerated. ExpD also shows that assimilating SST increases the error, especially under 300 m. The results for salinity are similar.

For SSH the largest improvement is achieved by assimilating SSH only (ExpB). The error against AVISO data in posterior state reduces by 26% from 8.9 cm to 6.6 cm (Fig. 9(A)). In the control run, the error is approximately 8 cm in most of the region, but in the southern part, it is about 13 cm. When SSH is assimilated, the error in the whole domain is low (5 cm) and uniform. In the 5-day forecast, ExpB still produces a lower error (7.0 cm) than the control run showing that the signal in SSH assimilation can last at least 5 days. When SST is assimilated alone, the error in the analysis (9.6 cm) is actually higher than in the control run, especially in the autumn and winter seasons. When both SSH and SST are assimilated, the error in the analysis (8.0 cm) is lower than the SST alone assimilation, but is still higher than the control run during the last 80 days.

3.2.3. *Balanced data assimilation*

The effect of the balance operator is tested in two experiments by assimilating SSH alone (ExpE) and with SST (ExpF). When only SSH is assimilated, the major constraint is the geostrophic balance. If SST is also assimilated, the hydrostatic balance also provides some correction. Compared with the original algorithm, the balance operator improves the SSH and temperature estimation. As shown in Fig 7 and 9, the RMSE of both SST and SSH in ExpE (SSH assimilation with the balance operator) is lower during most of the period. Although the difference of average error is marginal in ExpB and ExpE (6.57 and 6.50 cm for SSH; 0.85 and 0.81°C for SST, respectively), the improvement is more significant during some periods and can be as high as 0.2°C and 1 cm . Particularly, the SSH forecast error with the balance operator is smaller by 1-3 cm than the unbalanced approach, suggesting that a posterior state with compatible SSH and velocity field is necessary for a better SSH forecast.

As for the subsurface, assimilating SSH with the balance operator is an optimal way to improve the subsurface temperature profile. For example, compared to ExpB, the improvement of temperature in ExpE is as high as

476 0.12 °C for the upper 300 m. On the other hand, if SST is assimilated, even
 477 with the balance operator (ExpF), the SSH error is higher than ExpE. The
 478 error of salinity shows similar trend.

479 A major challenge facing ocean data assimilation and forecast is the sim-
 480 ulation of currents. The results demonstrate the benefit from the geostrophic
 481 balance. Assimilating SSH with the balance operator produces the most re-
 482 alistic surface currents while SST assimilation does not improve the currents.
 483 The model surface currents are compared against OSCAR 1/3° 5-day mean
 484 ocean currents due to the spatial and temporal coverage (Fig. 10). Without
 485 data assimilation, the half-year mean RMSE of the currents components u
 486 and v in the control run (ExpA) is 2.03 cm/s and 0.86 cm/s respectively. By
 487 using the original EAKF, the error of u and v decreases by 32% to 1.39 cm/s
 488 and 12% to 0.76 cm/s. When the balance operator is used, the error of u
 489 and v decreases by a further 27% to 1.02 cm/s and 23% to 0.59 cm/s. The
 490 performance of the balanced EAKF is thus the best among all three exper-
 491 iments and reduces the error by 40% to 50% compared to the control run.
 492 A comparison with the drifter derived surface currents gives similar results
 493 (Table. 3), although the error is much higher than for the domain average.

494 The spatial pattern of surface currents (Fig. 11) also demonstrates the
 495 advantage of the balance operator for the currents simulation. In the control
 496 run the model is able to capture the eastward coastal currents but the cur-
 497 rents are too strong and reach the east coast of the Great Australian Bight.
 498 In addition, an anticyclonic eddy is observed in the middle of the domain
 499 (127°E~130°E, 34°S~37°S) in the OSCAR dataset. The control run does not
 500 produce this eddy and the speed error is around 4cm/s in this region. When
 501 SSH is assimilated, even when the balance operator is not used, the over
 502 strong north boundary currents is weaker and more realistic. The assimi-
 503 lation also reproduces the anticyclonic eddy, and the assimilation with the
 504 balance operator (speed error ~2 cm/s) is more realistic than that without
 505 (speed error ~2.5 cm/s).

506 3.3. A case study with strong wind forcing

507 From 26 March 2007 to 27 March 2007, a storm passed the region, with
 508 a mean wind stress of 0.22 Pa and a maximum of 0.31 Pa. This process is of
 509 particular importance because the data assimilation cycle starts on 27 March
 510 2007. Therefore the prior state is strongly unbalanced because the storm cre-
 511 ates strong ageostrophic currents and the posterior state is also unbalanced.

Fig. 12 depicts the ageostrophic currents in SSH assimilations with and without balance operator in a subdomain significantly impacted by this storm (126°E~132°E, 34°S~37°S). The ageostrophic currents are stronger without balance operator (25.1 cm/s and 20.8 cm/s in ExpB and ExpE respectively). In the prior state (5-day forecast) on 01 April 2007, the ageostrophic currents reduce in both experiments but remain stronger in the unbalanced experiment (13.7 cm/s and 10.3 cm/s). The comparison between simulated SSH and the AVISO observation also shows that the balanced experiment is more realistic (figure not shown).

When compared with the OSCAR dataset, the domain-averaged error of the 5-day mean surface currents during this period with the balance operator (1.4 cm/s and 0.7 cm/s for u and v respectively) is much smaller than that without balance operator (2.1 cm/s and 1.1 cm/s for u and v respectively). Daily differences between these two experiments are up to 3.2 cm/s. However, the daily observations are not available to verify which experiment is better. This case study suggests that when the wind stress is large (e.g., greater than 0.2 Pa) and hence the ageostrophic currents are strong, the balance operator is essential for a better estimation of the surface currents.

4. Discussion

In this study, we assimilate surface observations in both an idealised and a real cases and reduce the imbalance caused by the data assimilation process. Numerical models are designed to be physically balanced so the forecast of each ensemble should be equilibrated. However the combination of observation and numerical model is not balanced so data assimilation introduces imbalance and spurious waves into the dynamical systems (e.g. Greybush et al., 2011; Kepert, 2009; Lorenc, 2003; Neef et al., 2006). Theoretically, the numerical model is able to remove the imbalance within a certain period but the effect of unbalanced waves has been shown to be important in this paper and other studies (e.g. Kepert, 2009; Neef et al., 2006). Several methods have been proposed to eliminate such waves. For example, by using a low-order idealised model, Neef et al. (2006) have demonstrated that the waves can be removed by increasing the ensemble size and decreasing the assimilation window, but it is usually difficult to do so in the high-dimensional GCMs.

Due to the small ensemble size, the covariance used in EnKFs is usually insufficient to represent the true relationship between state variables. Estimates of the background error covariance between substantially distant grid

548 points are often exaggerated when using a small ensemble size (Houtekamer
 549 and Mitchell, 1998). Therefore a localisation procedure is necessary. How-
 550 ever, localisation also causes spurious waves (e.g. Greybush et al., 2011;
 551 Lorenc, 2003) and thus is a main disadvantage of EnKFs.

552 Following Weaver et al. (2005), three physical balance constraints (temperature-
 553 salinity, hydrostatic and geostrophic balance) are used in this paper to reduce
 554 these spurious waves. We use an idealised shallow water model to reveal how
 555 the geostrophic balance operator enhances the data assimilation by removing
 556 the initial spurious ageostrophic waves. In this idealised model, the incre-
 557 ment is strongly unbalanced (Fig. 2) without the balance operator and the
 558 spurious waves persist more than 24 hours. The unrealistic ageostrophic cur-
 559 rents reduce the performance of data assimilation and therefore a balance
 560 operator is needed.

561 In the real case, the balance operator is also valuable in the estimation
 562 of ocean currents. Fig. 13 displays an example of the ensemble correlation
 563 between SST, SSH and surface and subsurface zonal ocean currents from
 564 a prior ensemble in the SSH only assimilation (ExpB). The correlation of
 565 surface variables with ocean currents is defined as,

$$\begin{aligned}
 C_{HUV} &= \sqrt{\frac{1}{2}(Corr(SSH, U)^2 + Corr(SSH, V)^2)} \\
 C_{TUV} &= \sqrt{\frac{1}{2}(Corr(SST, U)^2 + Corr(SST, V)^2)} .
 \end{aligned}
 \tag{12}$$

566 It is evident that in most of the region the correlation between surface
 567 observed variables and ocean currents is noisy and weak (less than 0.5 in most
 568 of the region). For the deeper currents, the correlation is slightly stronger,
 569 especially in the southern part. Further analysis (figure not shown) reveals
 570 that in the eastern part the currents are dominated by wind stress and the
 571 southern part features with stronger SSH variability. This could explain why
 572 EAKF and Ensemble Optimal Interpolation (EnOI) show good results in
 573 the Gulf of Mexico (Hoteit et al., 2013; Counillon and Bertino, 2009) where
 574 the SSH variability is dominated by the loop current and the correlation
 575 between SSH and surface currents is high (0.7 - 0.8, (Counillon and Bertino,
 576 2009)). However, in the Southern Australian Sea, the SSH variability is not
 577 constant and shows lower correlation with ocean currents. Thus EAKF gives
 578 worse currents result when only SSH is assimilated. Therefore the physical
 579 constraint is particularly important in this region.

580 The advantages of the balance operator have been shown in both an ide-
 581 alised shallow water model and the ROMS real case, in which the error of
 582 temperature, salinity, SSH and velocities reduces. Especially for the sub-
 583 surface temperature and salinity, when SSH is assimilated with the balance
 584 operator, the simulated error reduces dramatically in each layer. This indi-
 585 cates a better subsurface ocean circulation is produced. While SST is also
 586 assimilated, the error increases. This may be because the SST information in
 587 this region does not reflect the mesoscale ocean dynamics, which also seen in
 588 the unbalanced experiments. Compared with other approaches (e.g., using
 589 the streamfunction-velocity potential covariance, Kepert, 2009), the balance
 590 operator is straightforward and easy to compute and implement. In this
 591 work, the balanced part of sea surface height is approximated by integrating
 592 the density from a reference level. However, in regions where the bathymetry
 593 is complicated, that may be questionable. Another potential challenge of im-
 594 plementing the balance operator is that the mixed layer depth varies in time
 595 and space, but here we assign a constant value. Nevertheless, we anticipate
 596 this to be a minor correction.

597 **5. Conclusion**

598 An EnKF based ocean data assimilation system has been developed and
 599 applied to the South Australian Sea in this paper. This system applies the
 600 Ensemble Adjustment Kalman Filter (EAKF) in the Data Assimilation Re-
 601 search Testbed (DART) to the Regional Ocean Modeling System (ROMS).
 602 Spurious waves are created in the data assimilation process due to the local-
 603 isation and multivariate update scheme. We add a physical balance operator
 604 to this system to eliminate these spurious waves. The effect of the balance
 605 operator is demonstrated in a two dimensional shallow water model for differ-
 606 ent localisation scale. A larger localisation shows advantages over the smaller
 607 one. For both localisation scales, the balance operator decreases the error of
 608 sea surface height and velocities. It is also shown that the benefit of balance
 609 operator increases as the amplitude of SSH and wind stress increase.

610 SST and SSH are assimilated separately in a 10 km resolution ROMS
 611 model of the South Australian Sea, the error of SST and SSH reduces in
 612 the analysis. However, assimilating SST deteriorates the overall estimation
 613 of SSH, especially in the winter season. On the other hand, in the SSH
 614 assimilation experiment, the distribution of SST is similar to the control
 615 run. The assimilation of both SST and SSH is similar to just SST because

the number of SST observations is much higher than SSH. Assimilating SSH also improves the estimation of surface ocean currents. The balance operator is then used in the SSH only and SSH and SST assimilation experiments. The estimations of both SSH and temperature are improved, especially for the forecast, indicating a balanced posterior state is important. The balance operator is important in the estimation of ocean currents, assimilating SSH with the balance operator produces ocean currents the most comparable with OSCAR dataset. The error of u and v is reduced by 27% and 23% compared with the original data assimilation. The comparison with drifter derived surface currents shows similar results. The error of temperature profiles against Argo data suggests assimilating SSH with balance operator produces the most realistic subsurface temperature and salinity. A case study with a storm affecting this region shows that under high wind forcing condition the balance operator reduces the ageostrophic currents significantly in both analysis and forecast. The results in all experiments performed in this paper suggest that the balance operator may be useful to implement generally in ocean data assimilation systems.

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Experiment set	η_0 (cm)	τ_0 (Pa)	localisation scale (km)
A (fixed τ_0 amplitude)	5,10,20,30,40,50	0.1	60,100
B (fixed η_0 amplitude)	10	0.05,0.1,0.2,0.3,0.4,0.5	60,100

Table 1: Experiment design for the shallow water model

Experiment	Assimilated variables	Balance operator
ExpA (control run)	None	No
ExpB	SSH	No
ExpC	SST	No
ExpD	SSH and SST	No
ExpE	SSH	Yes
ExpF	SSH and SST	Yes

Table 2: Experiment design for the ROMS real case

	ExpA	ExpB	ExpC	ExpD	ExpE	ExpF
<i>SSH</i>	8.87	6.57	9.55	7.98	6.50	7.28
<i>SST</i>	0.86	0.85	0.36	0.37	0.81	0.33
<i>u</i>	25.80	20.73	23.79	23.81	19.52	21.40
<i>v</i>	21.32	19.23	23.13	22.35	18.19	20.73
<i>t</i> (100-300m)	1.18	1.04	1.06	0.94	0.92	0.99
<i>t</i> (300-700m)	1.15	1.13	1.22	1.14	1.06	1.12
<i>t</i> (700-1500m)	0.69	0.51	0.61	0.61	0.59	0.57
<i>s</i> (100-300m)	0.20	0.18	0.21	0.19	0.18	0.21
<i>s</i> (300-700m)	0.09	0.07	0.10	0.05	0.06	0.08
<i>s</i> (700-1500m)	0.13	0.12	0.14	0.12	0.12	0.13

Table 3: The RMSE of SSH, SST surface currents and subsurface temperature and salinity compared with AVISO, OISST, drifter and ARGO data. The units are cm, °C, cm/s, °C and PSU respectively.

Figure 1: A schematic description of the balanced data assimilation system.

Figure 2: A schematic description of the shallow water model.

Figure 3: Snapshots of A) SSH (contour) and velocities (quiver) from the unbalanced experiment, B) SSH and ageostrophic velocities from the unbalanced experiment and C) SSH and velocities from the balanced experiment. The units of SSH are cm.

Figure 4: RMSE of SSH (A and C) and meridional velocity v (B and D) with varying initial η amplitude (upper panel) and wind forcing (lower panel) in the idealised case.

Figure 5: ROMS simulated SST mean and standard deviation compared to OISST observation. The units are $^{\circ}\text{C}$. The crosses and dots in A) and C) represent the locations of ARGO floats and drifters.

Figure 6: The first 2 EOFs of deseasonalised (left panel) AVISO daily Sea Level Anomaly (SLA) data and (right panel) ROMS simulated SLA between 2006 and 2012. The units are cm.

Figure 7: ROMS simulated SST mean and standard deviation compared to OISST observation. The units are $^{\circ}\text{C}$.

Figure 8: RMSE of subsurface temperature vertical profile.

Figure 9: RMSE of SSH for A) posterior state (i.e., the analysis) and B) prior state (i.e., the 5-day forecast). The units are cm.

Figure 10: RMSE of top 30m A) zonal and B) meridional currents compared with OSCAR. The units are cm/s.

Figure 11: A comparison of top 30m currents of A) OSCAR dataset, B) ROMS control run, C) SSH assimilation without balance operator and D) SSH assimilation with balance operator

Figure 12: Snapshots of surface ageostrophic currents of posterior state on 27/03/2007 and prior state on 01/04/2007 in ExpB and ExpE

Figure 13: Ensemble correlations between surface variables and surface and subsurface currents on 30 January 2007 in ExpB. A) Correlation between SST and 5m currents, B) Correlation between SST and 200m currents, C) Correlation between SSH and 5m current, D) A) Correlation between SSH and 200m currents

894 **Appendix A. Representation of the linear balance operator and** 895 **background error covariance matrix**

896 As described in Section 2.1, each variable except T is decomposed into
897 unbalanced and balanced components and the balanced part is computed
898 from other variables using the linear balance operator L . The explanation of
899 L is given in this appendix.

900 Weaver et al. (2005) proposed to use 3 balance constraints, the tempera-
901 ture - salinity balance, hydrostatic balance and geostrophic balance for ocean
902 data assimilation, and the variables and their increments can be decomposed
903 as following,

$$904 \delta T = \delta T, \quad (\text{A.1})$$

$$905 \delta S = \delta S_B + \delta S_U = L_{ST}\delta T + \delta S_U, \quad (\text{A.2})$$

$$906 \delta \eta = \delta \eta_B + \delta \eta_U = L_{\eta\rho}\delta\rho + \delta \eta_U, \quad (\text{A.3})$$

$$\begin{aligned} \delta u &= \delta u_B + \delta u_U = L_{up}\delta p + \delta u_U \\ \delta v &= \delta v_B + \delta v_U = L_{vp}\delta p + \delta v_U \end{aligned} \quad (\text{A.4})$$

907 where

$$908 \delta\rho = L_{\rho T}\delta T + L_{\rho S}\delta S, \quad (\text{A.5})$$

$$\delta p = L_{p\rho}\delta\rho + L_{p\eta}\delta\eta. \quad (\text{A.6})$$

909 The first constraint (Eq. A.1) is the T - S relationship which regulates
910 the property of the water mass. It is based on the property of the prior
911 ensemble,

$$\delta S_B = r \frac{dS}{dz} \frac{dz}{dT} \delta T, \quad (\text{A.7})$$

912 where $r = 1 - e^{-z/z_M}$ is defined the same as in the ROMS-4DVAR (Moore
913 et al., 2011c) package, z is the vertical coordinate and z_M is the mixed layer
914 depth. The mixed layer depth is set to a constant value (200 m). In this
915 region, the mixed layer depth is between 50 m to 120 m but under some
916 extreme events (e.g., storms) it can be up to about 200 m. For a smaller ac-
917 tual mixed layer depth, this assumption will overweight the balanced salinity
918 below the mixed layer. The density (Eq. A.5) is a function of temperature
919 and salinity and is calculated using a linearised version of the equation of
920 state described by Jackett and McDougall (1995), where $L_{\rho T} = \rho_0 * \alpha$ and

921 $L_{\rho S} = \rho_0 * \beta$. The reference density ρ_0 is set to 1025 kg/m³ and α and β is
 922 the thermal expansion and saline contraction coefficients, respectively.

923 The second constraint is the hydrostatic balance which computes the
 924 balanced (baroclinic) sea level from the density and, therefore, temperature
 925 and salinity. The complete expression of the baroclinic relationship is an
 926 elliptic equation (Weaver et al., 2005),

$$\nabla \cdot H \nabla \delta \eta_B = -\nabla \cdot \int_{z=-H}^0 \int_{z'=z}^0 (\nabla \delta \rho(z') / \rho_0) dz' dz, \quad (\text{A.8})$$

927 where H is the ocean depth. Eq. A.8 excludes the influence of advection,
 928 assuming it is not important. However, this may be problematic in the areas
 929 where the contribution of advection is great such as the coastal region. To
 930 reduce the computational cost, a simplified version of Eq. A.8 is used in this
 931 paper by assigning a ‘depth of no motion’ z_0 (1000 m in this paper),

$$\delta \eta_B = \int_{z'=z_0}^0 (\delta \rho(z') / \rho_0) dz', \quad (\text{A.9})$$

932 and in regions where the ocean is shallower than z_0 Eq. A.9 is integrated
 933 from the bottom.

934 Then the pressure at depth z is computed by integrating the hydrostatic
 935 equation from z to the surface,

$$\delta p(z) = \int_{z'=z}^0 (\delta \rho(z') g) dz' + \rho_0 g \delta \eta, \quad (\text{A.10})$$

936 The third balance operator is the geostrophic balance, which computes
 937 the increments of u and v from sea level.

$$\begin{aligned} \delta u_B(z) &= -\frac{1}{\rho_0 f} \frac{\partial \delta p(z)}{\partial y} \\ \delta v_B(z) &= \frac{1}{\rho_0 f} \frac{\partial \delta p(z)}{\partial x} \end{aligned}, \quad (\text{A.11})$$

938 where f is the Coriolis force, x and y are the horizontal coordinates. The
 939 continuity constraint is not explicitly implemented, but it is satisfied above
 940 the depth of no motion because the balanced velocity is in geostrophic balance
 941 with η .

942 By using the above three balance constraints, the balanced component
 943 can be computed. In addition, we assume that the unbalanced components
 944 are uncorrelated with each other and thus the unbalanced error covariance
 945 is a block diagonal,

$$B_u = \begin{pmatrix} B_T & 0 & 0 & 0 & 0 \\ 0 & B_S & 0 & 0 & 0 \\ 0 & 0 & B_\eta & 0 & 0 \\ 0 & 0 & 0 & B_u & 0 \\ 0 & 0 & 0 & 0 & B_v \end{pmatrix}, \quad (\text{A.12})$$

946 where B_x is the error covariance of the unbalance component of variable x .
 947 The linear balance operator matrix is a lower triangular matrix

$$L = \begin{pmatrix} I & 0 & 0 & 0 & 0 \\ L_{ST} & I & 0 & 0 & 0 \\ L_{\eta T} & L_{\eta S} & I & 0 & 0 \\ L_{uT} & L_{uS} & L_{u\eta} & I & 0 \\ L_{vT} & L_{vS} & L_{v\eta} & 0 & I \end{pmatrix}, \quad (\text{A.13})$$

where,

$$\begin{aligned} L_{\eta T} &= L_{\eta\rho} L_{\rho T}, \\ L_{\eta S} &= L_{\eta\rho} L_{\rho S}, \\ L_{uT} &= L_{up} L_{p\rho} L_{\rho T}, \\ L_{uS} &= L_{up} L_{p\rho} L_{\rho S}, \\ L_{u\eta} &= L_{up} L_{p\eta}, \\ L_{vT} &= L_{vp} L_{p\rho} L_{\rho T}, \\ L_{vS} &= L_{vp} L_{p\rho} L_{\rho S}, \\ L_{v\eta} &= L_{vp} L_{p\eta}. \end{aligned}$$

948 Therefore the background error covariance matrix is,

$$LB_U L^T = \begin{pmatrix} B_{TT} & B_{ST}^T & B_{\eta T}^T & B_{uT}^T & B_{vT}^T \\ B_{ST} & B_{SS} & B_{\eta S}^T & B_{uS}^T & B_{vS}^T \\ B_{\eta T} & B_{\eta S} & B_{\eta\eta} & B_{u\eta}^T & B_{v\eta}^T \\ B_{uT} & B_{uS} & B_{u\eta} & B_{uu} & B_{vu}^T \\ B_{vT} & B_{vS} & B_{v\eta} & B_{vu} & B_{vv} \end{pmatrix}, \quad (\text{A.14})$$

where

$$\begin{aligned}
B_{TT} &= B_T, \\
B_{ST} &= L_{ST} B_T, \\
B_{\eta T} &= L_{\eta T} B_T, \\
B_{uT} &= L_{uT} B_T, \\
B_{vT} &= L_{vT} B_T, \\
B_{SS} &= L_{ST} B_T L_{ST}^T + B_S, \\
B_{\eta S} &= L_{\eta S} B_S, \\
B_{uS} &= L_{uS} B_S, \\
B_{vS} &= L_{vS} B_S, \\
B_{\eta\eta} &= L_{\eta T} B_T L_{\eta T}^T + L_{\eta S} B_S L_{\eta S}^T + B_\eta, \\
B_{u\eta} &= L_{uT} B_T L_{\eta T}^T + L_{uS} B_S L_{\eta S}^T + L_{u\eta} B_\eta, \\
B_{v\eta} &= L_{vT} B_T L_{\eta T}^T + L_{vS} B_S L_{\eta S}^T + L_{v\eta} B_\eta, \\
B_{uu} &= L_{uT} B_T L_{uT}^T + L_{uS} B_S L_{uS}^T + L_{u\eta} B_\eta L_{u\eta}^T + B_u, \\
B_{vu} &= L_{vT} B_T L_{uT}^T + L_{vS} B_S L_{uS}^T + L_{v\eta} B_\eta L_{u\eta}^T, \\
B_{vv} &= L_{vT} B_T L_{vT}^T + L_{vS} B_S L_{vS}^T + L_{v\eta} B_\eta L_{v\eta}^T + B_v.
\end{aligned}$$

949 This background error covariance matrix is used in all the balanced data
 950 assimilation experiments to compute the updated mean and covariance.

951 **Appendix B. Implementation of the linear balance operator in EAKF**

952 The EAKF algorithm (Anderson, 2001) is used in this work. The main
 953 difference of EAKF and the conventional EnKF is that in EAKF, an adjust-
 954 ment matrix A is used to compute the the posterior covariance so that

$$B^a = A^T B^f A, \quad (\text{B.1})$$

955 and the posterior state is

$$x^a = A(x^f - \overline{x^f}) + \overline{x^a}. \quad (\text{B.2})$$

956 In this work the adjustment matrix is the same with that described by An-
957 derson (2001, 2003) and Eq. B.2 becomes

$$x^a = AL_B(x_u^f - \overline{x_u^f}) + \overline{x^a}. \quad (\text{B.3})$$

958 In the balanced data assimilation experiments, the linear regression mul-
959 tivariate analysis procedure (Anderson, 2003) provided in DART is not used
960 and the unobserved variables is updated through Eq. B.3. This procedure
961 can only be performed in the model space so it is slower than the original
962 two-step EAKF algorithm.