The Regional Ocean Modeling System (ROMS) 4-dimensional variational data assimilation systems
Part III – Observation impact and observation sensitivity in the California Current System

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Abstract
The critical role played by observations during ocean data assimilation was explored when the Regional Ocean Modeling System (ROMS) 4-dimensional variational (4D-Var) data assimilation system was applied sequentially to the California Current circulation. The adjoint of the 4D-Var gain matrix was used to quantify the impact of individual observations and observation platforms on different aspects of the 4D-Var circulation estimates during both analysis and subsequent forecast cycles. In this study we focus on the alongshore and cross-shore transport of the California Current System associated with wind-induced coastal upwelling along the central California coast. The majority of the observations available during any given analysis cycle are from satellite platforms in the form of SST and SSH, and on average these data exert the largest controlling influence on the analysis increments and forecast skill of coastal transport. However, subsurface in situ observations from Argo floats, CTDs, XBTs and tagged marine mammals often have a considerable impact on analyses and forecasts of coastal transport, even though these observations represent a relatively small fraction of the available data at any particular time.

During 4D-Var the observations are used to correct for uncertainties in the model control variables, namely the initial conditions, surface forcing, and open boundary conditions. It is found that correcting for uncertainties in both the initial conditions and surface forcing has the largest impact on the analysis increments in alongshore transport, while the cross-shore transport is controlled mainly by the surface forcing. The memory of the circulation associated with the control variable increments was also explored in relation to 7 day forecasts of the coastal circulation. Despite the importance of correcting for surface forcing uncertainties during analysis cycles, the coastal transport during forecast cycles initialized from the analyses has less memory of the surface forcing corrections, and is controlled primarily by the analysis initial conditions.

Using the adjoint of the entire 4D-Var system we have also explored the sensitivity of the coastal transport to changes in the observations and the observation array. A single integration of the adjoint of 4D-Var can be used to predict the change that occurs when observations from different platforms are omitted from the 4D-Var analysis. Thus observing system experiments can be performed for each data assimilation cycle at a fraction of the computational cost that would be required to repeat the 4D-Var analyses when observations are withheld. This is the third part of a three part series describing the ROMS 4D-Var systems.

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1. Introduction

Critical components of any ocean data assimilation system are the observations, and a rigorous quantitative assessment of the
The impact of the observations on ocean circulation estimates derived from data assimilation should form an essential part of all modern data assimilation systems. In meteorology, the continuous monitoring of observation impacts on atmospheric analyses and forecasts has become common-place, and has demonstrated the importance of such activities both for data quality control and for assessing the efficiency of current observational networks and satellite platforms (e.g. Cardinalli, 2009). With the rapid expansion of ocean observing systems in recent years, similar monitoring efforts will doubtless prove valuable in oceanography.

In Moore et al. (in press a), hereafter referred to as Part I, we described in detail a suite of 4-dimensional variational (4D-Var) data assimilation systems that have been developed for the Regional Ocean Modeling System (ROMS), a widely used community ocean model (Haidvogel et al., 2008). The performance of the ROMS 4D-Var system was demonstrated in Moore et al. (in press b), hereafter referred to as Part II, in connection with the California Current System (CCS). In this third companion paper, we will demonstrate two additional capabilities of the ROMS 4D-Var system, namely observation impact and observation sensitivity. Observation impact calculations can be used to quantify the contribution of each individual datum to the difference between the background (or prior) and the analysis (or posterior) of some aspect of the ocean circulation. Observation sensitivity calculations, on the other hand, quantify the change that will occur in the circulation estimate as a result of changes in the observations or observation array. In addition to routine monitoring, observation impact calculations can provide quantitative information about systematic errors in the model in places or regions where the model is unable to reliably fit the observations. Similarly, observation impact calculations can demonstrate the influence of initialization shocks on the circulation that are associated with each individual datum. Observation sensitivity calculations, on the other hand, provide important information about the influence of data error and uncertainties on the circulation estimates, and are an efficient tool for observing system experiments (OSEs), offering also the potential for the design of observation arrays and adaptive sampling strategies.

The observation impact and observation sensitivity calculations presented here are based on the adjoint approach, and utilize the property of adjoint operators for identifying the subspace of the model state-vector that is activated by the observations. While adjoint-based methods have been used previously in oceanography in attempts to identify optimal observing locations and observation types (e.g. Köhl and Stammer, 2004; Zhang et al., 2010), our joint-based methods have been used previously in oceanography (see Checkley and Barth (2009) for a recent overview). A complete list of all symbols used and definitions can be found in Table 1 of Part I.

2. ROMS 4D-Var: a summary and notation

Following the notation introduced in Part I, we denote by \( \mathbf{x} \) the ROMS state-vector comprised of all the grid point values of temperature \( T \), salinity \( S \), velocity \( \mathbf{u} \), and free surface height \( \zeta \). Data assimilation seeks to combine in an optimal way a background (or prior) estimate of the circulation, \( \mathbf{x}^b(t) \), with observations which are arranged in the vector \( \mathbf{y} \). The background circulation is a solution of ROMS and depends on background estimates of the initial conditions, \( \mathbf{x}^b(t_0) \), surface forcing, \( \mathbf{F}(t) \), and open boundary conditions, \( \mathbf{b}(t) \). In 4D-Var the optimal (or “best”) circulation estimate is identified by adjusting a vector of control variables comprised of the initial conditions, surface forcing, open boundary conditions, and corrections for model error. In ROMS, 4D-Var is implemented using the incremental formulation of Courtier et al. (1994) in which the control vector, denoted \( \mathbf{d} \), is comprised of increments to the priors, specifically increments to the initial conditions, \( \mathbf{d}(t_0) \), surface forcing, \( \mathbf{d} \mathbf{F}(t) \), open boundary conditions, \( \mathbf{d} \mathbf{b}(t) \), and corrections for model error, \( \mathbf{d} \eta(t) \), for the data assimilation cycle starting at time \( t \). In the case of \( \mathbf{d} \), \( \mathbf{d} \mathbf{a} \) and \( \mathbf{d} \eta \), the increment \( \mathbf{d} \mathbf{z} \) contains information about these control vector increments at all times spanning the data assimilation window. If we denote the vector of background control variables as \( \mathbf{z}^b \), the best circulation estimate is given by \( \mathbf{z} = \mathbf{z}^b + \mathbf{d} \mathbf{z} \) where \( \mathbf{d} \mathbf{z} \) is the vector of analysis (or posterior) increments, and minimizes the cost function:

\[
J(\mathbf{d} \mathbf{z}) = \frac{1}{2} \mathbf{d} \mathbf{z}^T \mathbf{D}^{-1} \mathbf{d} \mathbf{z} + \frac{1}{2} (\mathbf{G} \mathbf{d} \mathbf{z} - \mathbf{d})^T \mathbf{R}^{-1} (\mathbf{G} \mathbf{d} \mathbf{z} - \mathbf{d})
\]

where \( \mathbf{D} \) and \( \mathbf{R} \) are the background and observation error covariance matrices respectively; \( \mathbf{G} \) is the tangent linear model sampled at the observation points; \( \mathbf{d} = \mathbf{y} - H(\mathbf{x}^b(t)) \) is the innovation vector; and \( H(\mathbf{x}^b(t)) \) is the background evaluated at the observation points via the observation operator \( H \).

The analysis increments can be expressed as \( \mathbf{d} \mathbf{z}^a = \mathbf{K d} \) where \( \mathbf{K} \) is the gain matrix, which can be written in two equivalent forms:

\[
\mathbf{K} = (\mathbf{D}^{-1} + \mathbf{G}^T \mathbf{R}^{-1} \mathbf{G})^{-1} \mathbf{G}^T \mathbf{R}^{-1}
\]

(2)

\[
\mathbf{K} = \frac{\mathbf{D} \mathbf{G}^T}{\mathbf{D} \mathbf{G}^T \mathbf{R}^{-1} \mathbf{G} \mathbf{D} + \mathbf{R}^{-1}}.
\]

(3)

Eq. (2) is sometimes referred to as the primal form of \( \mathbf{K} \) and arises from searching for \( \mathbf{d} \mathbf{z}^a \) in the full space spanned by the control vector \( \mathbf{d} \mathbf{z} \). Alternatively (3) is referred to as the dual form of \( \mathbf{K} \) and arises from a search for \( \mathbf{d} \mathbf{z}^a \) in the subspace of linear combinations of \( \mathbf{d} \mathbf{z} \) spanned only by the observations. Eq. (2) describes the
so-called incremental 4D-Var (4D-Var) approach used in ROMS, while (3) corresponds to the Physical-space Statistical Analysis System (4D-PSAS) and indirect representor 4D-Var (R4D-Var) approach which are also available in ROMS. In practice, none of the 4D-Var algorithms can be run to complete convergence, in which case \( \delta z' = Kd \) where \( K \) is referred to as the practical gain matrix, and is a reduced rank approximation of \( K \).

For later reference, we also adopt from Part I the following operators: the tangent linear model \( M \) such that \( \delta x(t_1) = M(t_0, t_{-1}) \delta x(t_{-1}) \) where \( \delta x(t_{-1}) = (\delta x(t_{-1}), \delta \tilde{f}(t_1), \delta \tilde{b}(t_1), f'(t_1))^T \), and the tangent linear operator \( M(t_0, t_0) \) which isolates the state-vector increment \( \delta x(t_0) \) given the control vector increment \( \delta z \), according to \( \delta x(t_0) = M(t_0, t_0) \delta z \). The corresponding adjoint equations are \( \delta \tilde{x}'(t_{-1}) = M'(t_{-1}, t_0) \delta p(t_0) \) and \( \delta x' = M'(t_0, t_0) \delta p(t_0) \) where \( p(t_0) \) is the adjoint state-vector. For mathematical convenience, we often wish to isolate the tangent linear circulation \( \delta x \) that can be attributed to only specific elements of the control vector \( \delta z \). In the case of the contribution of the initial conditions to \( \delta x(t_0) \) we have \( \delta x(t_0) = M(t_0, t_0) J_{0m} \delta x(t_{-1}) \) where \( J_{0m} = (I_{nm} 0) \) was introduced in the appendix of Part I; \( I_{nm} \) is the \((n_m \times n_m)\) identity matrix; \( 0_m \) is the null matrix of dimension \((n_m \times (N - K)(n_y + n_z))\); and \( n_m, n_y \) and \( n_z \) are the dimensions of the vectors \( \delta x(t) \) (and \( f'(t) \)), \( \delta \tilde{f}(t) \) and \( \delta \tilde{b}(t) \) respectively and \( N \) is the number of timesteps in the assimilation interval. Similar \( J \) operators can be defined that map \( \delta f, \delta b \) and \( \delta f'(t) \) into state-space, but they are not required here.

### 3. Model and 4D-Var configuration

The configuration of ROMS and 4D-Var used in the calculations reported below is described in detail in Part II and by Broquet et al. (2009a,b, 2011), so only a brief description will be given here.

The ROMS CCS domain spans the region 134°W to 116°W and 31°N to 48°N, with 10 km horizontal resolution and 42 terrain following \( \sigma \)-levels in the vertical. This is the model referred to in Part II as WC10, and for consistency we shall use the same notation here also. WC10 provides reasonable resolution of the CCS mesoscale circulation features, and at the same time represents a computational challenge for 4D-Var. The model domain and bathymetry are shown in Fig. 1.

The model forcing was derived from daily averaged output of atmospheric boundary layer fields from the Naval Research Laboratory’s (NRL) Coupled Ocean–Atmosphere Mesoscale Prediction System (COAMPS\( ^\text{®} \)) (Doyle et al., 2009) using the bulk formulations of Liu et al. (1979) and Fairall et al. (1996a,b). The resulting surface fluxes of momentum, heat, and freshwater represent the background surface forcing, denoted \( F(t) \) in Section 2. The model domain has open boundaries at the northern, southern, and western edges where the tracer and velocity fields were prescribed, and the free surface and vertically integrated flow were subject to Chapman (1985) and Flather (1976) boundary conditions respectively. The prescribed open boundary solution was taken from the Estimating the Circulation and Climate of the Ocean (ECCO) global data assimilation product (Wunsch and Heimbach, 2007), and represents the background boundary conditions denoted \( b(t) \) in Section 2. A sponge layer was also used adjacent to each open boundary in which viscosity increased linearly from \( 4 \text{ m}^2 \text{s}^{-1} \) in the interior to \( 100 \text{ m}^2 \text{s}^{-1} \) at the boundary over a distance of \( \sim 100 \text{ km} \).

As in Part II, ROMS 4D-Var was run sequentially starting from a background initial condition on 27 July 2002 derived from the 4D-Var sequence of Broquet et al. (2009a). The observations assimilated in the model were collected by various platforms, and include: gridded sea surface height analyses in the form of dynamic topography from Aviso at \( \sim 1/3^\circ \) resolution every 7 days; a blended SST product with 10 km resolution, available daily, and consisting of 5 day means derived from the GOES, AVHRR and MODIS satellite instruments (available east of \( 130^\circ \)W only at the time the experiments presented here were performed); \( \text{in situ} \) hydrographic observations extracted from the quality controlled EN3 data archive (version v1b) maintained by the UK Met Office as part of the European Union ENSEMBLES project (Ingleby and Huddleston, 2007); and temperature observations made by tagged elephant seals as part of the Tagging of Pacific Pelagics program (TOPP). To reduce data redundancy, all observations within each model grid cell, over a 6 h time window, were combined to form “super observations,” and the standard deviation of the observations that contribute to the super observation in each grid cell was used as an estimate of the error of representativeness.

Observation errors were assumed to be uncorrelated in space and time, resulting in a diagonal observation error covariance matrix, \( R \). The variances along the main diagonal of \( R \) were assigned as a combination of measurement error and the error of representativeness. Measurement errors were chosen independent of the data source, with the following standard deviations: 0.02 m for dynamic topography; 0.4°C for SST; 0.1°C for \( \text{in situ} \) T; and 0.01 for \( \text{in situ} \) S.

A background error standard deviation associated with \( \chi'(t_0) \), \( f'(t) \) and \( b'(t) \) was estimated for each calendar month as follows. The background error standard deviations for the unbalanced initial condition components of the control vector were estimated based on the variance of the model run during the period 1999–2004 subject only to surface forcing (i.e. no data assimilation). The temporal variability of the COAMPS surface forcing for the period 1999–2004 was used as the variance for the background surface forcing error, and the open boundary condition background error variances were chosen to be the variances of the ECCO fields at the boundaries. In all of the experiments presented here, the circulation estimates were computed subject to the strong constraint, in which case model errors were assumed to be zero. At the present time, as noted in Parts I and II, ROMS 4D-Var supports only homogeneous error correlations that are separable in the horizontal and vertical. The decorrelation length scales used to model the background errors of all initial condition control variable components of \( D \) were 50 km in the horizontal and 30 m in the vertical. Horizontal correlation scales chosen for the background surface forcing error components of \( D \) were 300 km for wind stress and 100 km for heat and freshwater fluxes. The correlation lengths for the background open boundary condition error components of \( D \) were chosen to be 100 km in the horizontal and 30 m in the vertical. Explicit temporal correlations of the background errors

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**Fig. 1.** ROMS CCS model domain and bathymetry. Also shown are the 37°N and 500 m isobath sections across which the alongshore and cross-shore transports were computed.
are not currently considered in the current version of ROMS 4D-Var. However, the surface forcing and boundary condition increments, \( \delta f(t) \) and \( \delta b(t) \), were only computed daily (the same frequency as the daily averaged COAMPS data) and interpolated to each intervening model time step, a procedure which effectively introduces some temporal correlation of the errors in \( \mathbf{f}'(t) \) and \( \mathbf{b}'(t) \). A discussion of the choice of the aforementioned background error covariance parameters can be found in Broquet et al. (2009a,b, 2011) and Part II. In all of the calculations presented here, the multivariate balance operator, \( K_n \) (or the \( T-S \) sub-component of \( K_n \)) described in Part I (Section 5.2) was used.

4. CCS 4D-Var

4.1. Sequential strong constraint 4D-Var

To demonstrate the observation impact capabilities of ROMS, 4D-Var was run sequentially for the period July 2002–December 2004. Because of the uncertainty in assigning model error, all experiments presented here assume the strong constraint, although there is nothing to preclude the same computations using the weak constraint instead. In all cases, the control vector \( \mathbf{a} \) was comprised of increments to the initial conditions, surface forcing, and open boundary conditions. The background initial conditions \( \mathbf{x}^0(t_0) \) at the start of each assimilation cycle were chosen to be the analysis at the end of the previous assimilation cycle. The background surface forcing and open boundary conditions, however, are always those taken from COAMPS and ECCO. 4D-Var was run with 1 outer-loop and 10 inner-loops spanning 7-day assimilation cycles. As shown by Broquet et al. (2009a,b, 2011) and in Part II (Fig. 3b) this is enough to guarantee a significant level of convergence of the cost function \( J \) toward its minimum value. The ratio of the final and initial values of \( J \) for each assimilation cycle are shown in Fig. 2 which shows that \( J \) is typically reduced by a factor of 3 during each cycle.

Our focus here is on the circulation of the central California coast, characterized by energetic mesoscale variability, and by pronounced seasonal upwelling driven by alongshore wind stress and offshore wind stress curl. Upwelling favorable winds exist year round equatorward of about 40°N (Cape Mendocino), although upwelling is most intense during the spring and early summer. As upwelling intensifies, pronounced changes in the circulation occur, including the development of a nearshore coastal jet driven by the offshore pressure gradient that accompanies the coastal upwelling. In addition, the central California coastal circulation is the site of elevated eddy energy compared to sites further north (Kelly et al., 1998). The challenge for 4D-Var is to therefore build reliable estimates of the actual ocean conditions in this highly dynamic region, particularly during the seasonal transitions which can be very rapid and when the timing of the transitions varies from year-to-year.

Broquet et al. (2009a) demonstrated that 4D-Var yields significant changes in the central California coastal circulation, and Broquet et al. (2011) showed that the geostrophic component of the resulting estimates compares favorably with direct estimates from observations. In addition, Broquet et al. (2009a) found that ROMS vertical profiles of \( T \) and \( S \) in the central California region arising from 4D-Var compare well with independent observations that were not assimilated into the model. In this case, most of the observations that were assimilated were collected from repeat sampling arrays off the coast of Oregon and the Southern California Bight, both far from the central California region, which demonstrates the ability of 4D-Var to dynamically interpolate information from remotely sampled observations.

In order to quantify the impact of the available ocean observations and data assimilation on the circulation, we considered two measures of the transport as quantitative indicators of the major circulation changes that occur in the central California region, namely: (i) the alongshore transport across 37°N, and (ii) the transport in the upper 15 m of the water column crossing the continental shelf break, taken here as the 500 m isobath, between 35°N and 40.5°N. Both transport sections are indicated in Fig. 1. The latter was also analyzed by Veneziani et al. (2009) and is associated with variations in coastal upwelling due to coastal divergence driven by Ekman transport and Ekman pumping driven by wind stress curl. The observation impact and sensitivity calculations presented here therefore provide quantitative information about the observability of the transports associated with the seasonal upwelling circulations, and the ability of 4D-Var to dynamically interpolate information from the observations through the model domain.

4.2. Analysis cycle transport increments

The time average transport crossing 37°N in the upper 500 m during each analysis cycle was considered and can be expressed as

\[
\mathcal{J}_{37N}(x) = \sum_{i=1}^{2} \left( \mathbf{h}_{37N} \right) \mathbf{x}_i
\]

where \( [t_0, t_0 + \tau] = [k_1 \Delta t, k_2 \Delta t] \) is the time interval spanned by each assimilation cycle with \( \tau = 7 \) days in the experiments considered here, and \( \Delta t \) is the model time step; \( \mathbf{x}_i = \mathbf{x}(k_1 \Delta t) \) and \( \left( \mathbf{h}_{37N} \right) \) is a vector comprised of zero elements except for those elements that correspond to the velocity gridpoints that contribute to the transport normal to the 37°N section over the upper 500 m from the coast to 127°W (cf. Fig. 1). Similarly, we also considered the time average transport crossing the continental shelf break, which is defined as the 500 m isobath, given by

\[
\mathcal{J}_{500m}(x) = \sum_{i=1}^{2} \left( \mathbf{h}_{500m} \right) \mathbf{x}_i
\]

where \( \left( \mathbf{h}_{500m} \right) \) is a vector comprised of zero elements except for those elements that correspond to grid points in the upper 15 m (<8 uppermost vertical \( \sigma \)-levels) that contribute to the transport crossing the 500 m isobath between 35°N and 40.5°N. The \( \mathcal{J}_{500m} \) transport will be primarily due to the Ekman transport (Veneziani et al., 2009). The non-zero elements of

Fig. 2. Time series of the ratio of the final (\( J_f \)) and initial (\( J_i \)) values of the cost function \( J \) for each cycle of I4D-Var using WC10 with 1 outer-loop and 10 inner-loops (red curve), and R4D-Var using WC30 with 1 outer-loop and 50 inner-loops (blue curve) (see Section 6.1.2). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
Fig. 3 and b show time series of $J_{37N}(x^b)$ and $J_{500m}(x^c)$ for the background circulation estimate ($x^b$) for each 7 day 4D-Var assimilation cycle using WC10. In the case of $J_{37N}(x^b)$, the transport varies between 4 Sv poleward and 8 Sv equatorward, and is characterized by variability on seasonal and shorter timescales with a standard deviation of 3 Sv. The transport crossing the 500 m isobath is generally offshore (the convention used here is that $J_{500m}>0$ represents offshore transport) with a mean of $\approx 0.5$ Sv, standard deviation of 0.5 Sv, and peak values during spring and summer of $\approx 1.5$ Sv, although during winter $J_{500m}$ is close to zero.

The time averaged alongshore and cross-shore transports of the 4D-Var analyses, $x^a$, are given by $J_{37N}(x^a)$ and $J_{500m}(x^c)$ respectively and differ significantly from the background estimates. The circulation analysis increment at any time within the data assimilation window $[t_0, t_0 + 7]$ of each 4D-Var cycle is given

$$\Delta J = J(x^c) - J(x^b) = (k_2 - k_1)^{-1} \sum_{k=k_1}^{k_2} \mathbf{h}_k \mathcal{M}_b(t_k, t_0) \delta x^a$$

where $\mathcal{M}_b(t_k, t_0)$ denotes the tangent linear model (referred to as TLROMS) linearized about the background circulation. The approximate equality applies when the analysis increments $\delta x^a$ are small, in which case the transport increments during each assimilation cycle can be expressed as:

$$\Delta J = J(x^c) - J(x^b) = (k_2 - k_1)^{-1} \sum_{k=k_1}^{k_2} \mathbf{h}_k \mathcal{M}_b(t_k, t_0) \delta x^a$$

$$= (k_2 - k_1)^{-1} \sum_{k=k_1}^{k_2} \mathbf{h}_k ((\delta x^a)_k + (\delta x^c)_k + (\delta x^c)_k)$$

where $\mathcal{M}_b$ denotes either $J_{37N}(x)$ or $J_{500m}(x)$, and $\mathbf{h}$ represents either $h_{37N}$ or $h_{500m}$. In (5), the vectors $(\delta x^a)_k$, $(\delta x^c)_k$, and $(\delta x^c)_k$ represent the contributions to the time-evolving analysis increment of the

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**Fig. 3.** Time series of the 7 day average background (prior) transport from WC10 (a) across 37°N ($J_{37N}(x^b)$), and (b) crossing the 500 m isobath in the upper 15 m of the water column ($J_{500m}(x^c)$). Note that in (b) the convention used here is that values $>0$ represent offshore transport associated with coastal upwelling. Time series of the analysis (posterior) transport increments are shown in (c) across 37°N ($\Delta J_{37N}$), and (d) crossing the 500 m isobath ($\Delta J_{500m}$). The red curves represent the transport increments computed directly from the analysis and background circulation estimates of NLROMS, while the green curves show the increments computed using the tangent linear assumption (4). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
4D-Var increments in the initial conditions, surface forcing, and open boundary conditions, respectively.

Fig. 3c and d show time series of the transport increments $\Delta J_{\text{37N}}$ and $\Delta J_{\text{500m}}$ from WC10 for each 4D-Var assimilation cycle from two independent calculations: in one case the $\Delta J$ were computed directly from the difference between the analysis and background circulation estimates of the nonlinear ROMS (referred to as NLROMS), while in the other case the $\Delta J$ were computed using the tangent linear assumption of (4). The two time series agree very well for both $\Delta J_{\text{37N}}$ and $\Delta J_{\text{500m}}$, indicating that the tangent linear assumption is valid during each 7 day assimilation cycle. The alongshore (cross-shore) transport increments of Fig. 3c (Fig. 3d) have a mean of $-0.18 \text{ Sv} \ (-0.02 \text{ Sv})$ and are highly variable with a standard deviation of $0.46 \text{ Sv} \ (0.08 \text{ Sv})$.

Eq. (5) shows that the transport increments can be decomposed into the individual contributions from the 4D-Var increments $\delta x(t_0), \delta f(t)$ and $\delta b(t)$. Time series of the individual contributions to $\Delta J_{\text{37N}}$ and $\Delta J_{\text{500m}}$ are shown in Fig. 4 for each 4D-Var cycle of WC10. In the case of $\Delta J_{\text{37N}}$, Fig. 4a shows that there are clearly times when the increments in the initial conditions dominate, and times when the increments to the surface forcing are the primary factor controlling $\Delta J_{\text{37N}}$. During some cycles, the changes in $\Delta J_{\text{37N}}$ associated with the increments $\delta x(t_0)$ and $\delta f(t)$ are opposed. The rms over all cycles indicates that on average $\delta x(t_0)$ contributes more than $\delta f(t)$ to $\Delta J_{\text{37N}}$, while the impact of $\delta b(t)$ is generally small.

In the case of $\Delta J_{\text{500m}}$ (Fig. 4b), $\delta f(t)$ dominates and during several cycles $\delta x(t_0)$ opposites $\delta f(t)$, while $\delta b(t)$ impacts on $\Delta J_{\text{500m}}$ are negligible.

4.3. Forecast cycle transport and ocean memory

The impact of $\delta x(t_0), \delta f(t)$ and $\delta b(t)$ during each 4D-Var analysis cycle on forecasts of the transports $J_{\text{37N}}$ and $J_{\text{500m}}$ initialized from the analyses is also of interest and provides information about the memory of the circulation. Fig. 5 shows a schematic of overlapping 7 day analysis cycles and 14 day forecast cycles when 4D-Var is run sequentially as described in Section 3, where the forecasts are initialized from the best estimate circulations at the end of each analysis cycle. The interval spanned by analysis cycle $j$ is $[t_0, t_0 + 7]$, while the interval spanned by forecast cycle $j$ is $[t_0 + 7, t_0 + 14]$. We will focus here on the time interval $[t_0, t_0 + 14]$. The 14 day forecast that starts on day $t_0$ corresponds to forecast cycle $j - 1$ and will be referred to as $x_{j-1}^f$. Forecast cycle $j$ starts on day $t_0 + 7$, and the first 7 days $[t_0 + 7, t_0 + 14]$ of this forecast overlap the last 7 days of $x_{j-1}^f$. We will refer to the first 7 overlapping days of forecast cycle $j$ as $x_j^f$, where the final day of $x_j^f$ and $x_{j-1}^f$ verify at the same time, namely $t_0 + 14$. However, $x_j^f$ contains information from the observations assimilated during analysis cycle $j$, so our interest here lies in evaluating the impact of these observations on the skill of the 7 day forecast $x_j^f$ compared to the skill of the 14 day forecast $x_{j-1}^f$ at time $t_0 + 14$.

Specifically, we considered the impact of the observations on the skill of forecasts of alongshore and cross-shore transport. In the following experiments we considered forecasts of the transport averaged over the last day of forecast cycle $j - 1$, namely $[t_0 + 13, t_0 + 14]$ computed from $x_{j-1}^f$ and $x_{j-1}^b$, so that:

$$ J_j^f = (k_4 - k_3)^{-1} \sum_{k=k_3}^{k_4} \mathbf{h}_k^f (x_j^f) $$

(6)

where $J_j^f$ denotes either the forecast in alongshore transport ($J_j^f$), or cross-shore transport ($J_j^f$), $\tau = 7$ or 14 and corresponds to the duration of the forecasts $x_j^f$ and $x_{j-1}^f$, and $k_3 \Delta t = t_0 + 13$ and $k_4 \Delta t = t_0 + 14$. The times referenced by $k_2, k_3$ and $k_4$ in (6) are also indicated in Fig. 5. The summation in (6) is over the entire forecast verification time interval $[t_0 + 13, t_0 + 14]$, where $\mathbf{h}_k$ denotes either $(h_{37N}, h_{500m})$ or $(h_{500m}, h_{37N})$, and $\mathbf{h}_k = 0$ outside this interval.

If $x_0$ represents the true ocean circulation, and $J_0^f$ and $J_{-1}^f$ are the true time averaged transports, then the squared errors in the 7
and 14 day transport forecasts are given by \((\varepsilon_{37N})_j = \left( \mathcal{J}_{37N} \right)_j^2\) and \((\varepsilon_{500m})_j = \left( \mathcal{J}_{500m} \right)_j^2\). A measure of the impact on the transport forecast error of the observations assimilated during analysis cycle \(j\) spanning \(t = [t_0^j, t_0^j + 7]\) is \(\Delta \varepsilon_{37N}\).

Since the true circulation is not known, it is reasonable to use the verifying analysis \(\mathbf{x}_f^j\) of analysis cycle \(j + 1\) for the interval \(t = [t_0^j + 7, t_0^j + 14]\) as a surrogate for the truth (Langland and Baker, 2004). The justification for this approach in the present case is illustrated in Fig. 6 which shows time series of \((\mathbf{y}^j - \mathbf{y}_m)^T \mathbf{R}^{-1} (\mathbf{y}^j - \mathbf{y}_m)\), the weighted sum of the squared differences between the observations \(\mathbf{y}^j\) and the model circulation \(\mathbf{y}_m\) evaluated at the observation points. Three different cases are shown corresponding to \(\mathbf{y}_m\) sampled from \(\mathbf{x}_{14}^j\), \(\mathbf{x}_7^j\), and the verifying analysis \(\mathbf{x}_f^j\). Fig. 6 indicates that in general \(\mathbf{x}_7^j\) is closer to the observations than \(\mathbf{x}_{14}^j\), and for all forecast cycles the verifying analysis is best of all. However, Fig. 6 may present an over-optimistic picture since while both forecasts may not deviate much from the new observations sampled at repeat locations (e.g. satellite observations), they may actually be further from the truth elsewhere.

Unfortunately, truly independent observations are not available with which to validate the forecasts. Nonetheless, using \(\mathbf{x}(t)\) as a surrogate for \(\mathbf{x}(t)\) and using (6) we have:

\[
e_\tau = (k_4 - k_3)^{-2} \sum_{k=k_4}^{k_3} (\mathbf{x}_j^k - \mathbf{x}_f^j)^T \mathbf{h} \mathbf{h}^T (\mathbf{x}_j^k - \mathbf{x}_f^j)
\]

where \(e_\tau\) denotes \((\varepsilon_{37N})_\tau\) or \((\varepsilon_{500m})_\tau\), and as before \(\tau\) denotes the duration of the forecast (7 or 14 days). Recall from Fig. 5 that \(\mathbf{x}_{14}^j(t)\) and \(\mathbf{x}_f^j(t)\) overlap during the period \([t_0^j + 7, t_0^j + 14] = [k_4 \Delta t, k_4 \Delta t]\), so that we can write \(\mathbf{x}_j^k(t) = \mathbf{x}_{14}^j(t) + \delta \mathbf{x}(t)\). The contribution of the 4D-Var increments and observations to \(\Delta \varepsilon_{37N}\) and \(\Delta \varepsilon_{500m}\) can be evaluated by expanding (7) in terms of \(\delta \mathbf{x}(t)\) in order to obtain an explicit approximation \(\Delta e_\tau\) for \(\Delta e\) in terms of the forecast difference \(\delta \mathbf{x}(t)\). Errico (2007) discusses first-, second-, and third-order Taylor expansions for \(\Delta e\), and Gelaro et al. (2007) have demonstrated that in a numerical weather prediction model, the
second- and third-order expansions are superior to first-order in terms of the agreement between \( \delta e \) and direct computation of \( \delta e \) using the nonlinear forecast model. While the second- and third-order approximations are formally nonlinear in \( \delta x(t) \), Gelaro et al. (2007) show that they both produce results that are consistent with the linear first-order approximation. Experiments with WC30 (not shown) confirm these findings so in sequel we use a second-order expansion of (7) in terms of \( \delta x(t) \), in which case:

\[
\delta e = (k_4 - k_2)^{-2} \left( J^4 - J^2 \right) \sum_{j=1}^{k_4} h_j^4 (M_{14}) + \left( J^4 - J^2 \right) \times \sum_{j=1}^{k_4} h_j^2 (M_{14}) \int_0^{t_0+7} (\delta x(t_0 + 7) \right)
\]

where \( J^4 \) is the transport of the verifying analysis, \( M_{14} \) denotes TLROMS linearized about \( x_i^j(t_0) \); \( h_{37N} \) or \( h_{500m} \); the matrix \( J_0 \) was introduced in Section 2; and \( \delta x(t_0 + 7) \) is the state-vector analysis increment for the 4D-Var analysis cycle \( j \) ending on day \( t_0 + 7 \). It is important to note in (8) that even though the summations only span the interval \( [k_2 \Delta t, k_4 \Delta t] \), the integrations of TLROMS described by \( M_{14} \) start at \( k_2 \Delta t = t_0 + 7 \).

Fig. 7 shows time series of \( \Delta e \) and \( \delta e \) for 37\(^\circ\)N transport and 500 m isobath transport. In the case of \( \Delta e_{37N} \), Fig. 7a indicates that \( \delta e_{37N} \) agrees very well with the actual error \( \Delta e_{37N} \), and during 61% of the forecast cycles \( \delta e_{37N} < 0 \) indicating that \( x_i^j \) is closer than \( x_i^j \) to the transport of the verifying analysis. In the case of \( \Delta e_{500m} \) (Fig. 7b), \( \delta e_{500m} \) and \( \Delta e_{500m} \) sometimes disagree substantially. However, most cycles the agreement is very good, and for cycles when \( \delta e_{500m} \) significantly under-estimates \( \Delta e_{500m} \), the sign of the transport error difference is generally correct. Similarly, \( \delta e_{500m} < 0 \) for 63% of the cycles, indicating that on average assimilating observations improves the 7 day forecast skill of cross 500 m isobath transport.

The analysis increment \( \delta x(t_0 + 7) \) can also be decomposed into the contributions from the 4D-Var increments \( \delta x(t_0), \delta x(t) \) and \( \delta b(t) \) from the analysis cycle spanning the interval \( [t_0, t_0 + 7] \), which are shown for \( \delta e_{37N} \) and \( \delta e_{500m} \) in Fig. 8 for each forecast cycle. In both cases the contribution of the 4D-Var initial condition increments at \( t_0 \) dominate \( \delta e \) during the forecast verification time interval \( [t_0 + 13, t_0 + 14] \), although during some cycles the forcing increments are also a significant controlling factor. A comparison of the relative contributions of the 4D-Var control vector increments to \( \delta e \) in Fig. 8 with those of \( \Delta e \) in Fig. 4 gives information about the memory of the forecast circulation arising from \( \delta x(t_0), \delta x(t) \) and \( \delta b(t) \). Both the \( \delta x(t_0) \) and \( \delta b(t) \) components of \( \delta x \) exert considerable control on the alongshore and cross-shore transport analyses (Fig. 4). However, during ensuing forecast cycles initialized from \( M(t_0 + 7, t_0) \) (\( \delta x + \delta b \)), the errors \( \delta e_{37N} \) and \( \delta e_{500m} \) are largely controlled by the \( \delta x(t_0) \) component of \( \delta x \) indicating that the circulation has a longer memory of corrections made to the background initial conditions \( x_i^j(t_0) \) than corrections made to \( f(t) \) over the same analysis cycle. The fact that much of the forecast error is governed by the initial conditions of the 4D-Var analysis cycle, suggests a number of possibilities. The first inference is that the intrinsic hydrodynamic properties of the circulation (such as instabilities) are the primary factor controlling the development of forecast errors as opposed to errors in the surface forcing or open boundary conditions. Second, because of the relatively short analysis and forecast cycles (7–14 days), state estimation and prediction becomes primarily an initial value problem. In either case, good estimates of \( x_i^j(t_0) \) are required to make reliable forecasts of transport. In addition though, during the experiments presented here, the surface forcing and open boundary conditions during the verifying analysis and forecast intervals are identical, which may over emphasize the importance of initial condition errors. The impact of uncertainties in the initial forcing conditions, surface forcing, and open boundary conditions on the predictability of the circulation is explored further and in more detail by Moore et al. (submitted for publication).

5. Analysis-forecast cycle observation impacts

As described in Part I (Section 7.2), the impact of each observation on \( \Delta e \) in (4) can also be computed during analysis and forecast cycles. Specifically, for the case of a single outer-loop, the
change in $J(t)$ due to assimilating the observations is given to first-order by

$$
J(x^*(t)) - J(x(t)) = \Delta J(t) \approx d^T K' \mathcal{M}_t^{(k)} \mathcal{M}_t^{(k)} \mathcal{J} / \mathcal{V} \mathcal{h}_k,
$$

where $\mathcal{M}_t^{(k)} \mathcal{J} / \mathcal{V} \mathcal{h}_k$ denotes the time convolution of $\mathcal{J} / \mathcal{V} \mathcal{h}_k$ with the adjoint of ROMS linearized about the prior circulation; $d = y - H(x(t))$ is the innovation vector; and $K$ is the practical gain matrix introduced in Part I (Section 7.1). The contribution of each observation to the dot-product defining $\Delta J(t)$ can be readily computed using ROMS 4D-Var output. For cases involving more than one outer-loop, the second derivative of the nonlinear model $M$ is formally required to account for changes in $\Delta J(t)$ that arise from changes in the solution trajectory about which $\mathcal{M}_t^{(k)}$ is linearized. While the second derivative of $M$ is not available, Trémolet (2008) argues that linearizing $\mathcal{M}_t^{(k)}$ about the 37N isobath introduced in Section 4.

In the following subsections, we will explore the impact of the observations during each 4D-Var analysis-forecast cycle on the alongshore transport crossing 37N and the transport across the 500 m isobath introduced in Section 4.

5.1. 37°N transport analysis

The transport increments during each 4D-Var analysis cycle are given by (4) and (5). The analysis increment can also be written as

$$
\delta x^*(t) = \mathcal{M}_t(t, t_0) \delta z^*,
$$

where $\delta z^* = Kd$, in which case (4) can be expressed as follows:

$$
\Delta J = \mathcal{J}'(x^*) - \mathcal{J}'(x) \approx (k_2 - k_1)^{-1} d^T K' \mathcal{M}_t^{(k)} \mathcal{M}_t^{(k)} \mathcal{J} / \mathcal{V} \mathcal{h}_k
$$

$$
= d^T g = d^T (g_x + g_f + g_b)
$$

$$
= \sum_{i=1}^{N} d_i g_i = \sum_{i=1}^{N} d_i (g_x(i), g_f(i), g_b(i))
$$

where $(\mathcal{M}_t^{(k)})_k \equiv \mathcal{M}_t(k, \Delta t, k, \Delta t)$; the $d_i$ are the elements of the innovation vector $d$; and $g_i$ are the elements of $g = (k_2 - k_1)^{-1} K' \mathcal{M}_t^{(k)} \mathcal{M}_t^{(k)} \mathcal{J} / \mathcal{V} \mathcal{h}_k$. As in (10) and (11), the vector $g$ can be subdivided into the contributions from the 4D-Var increments in initial conditions $g_x = ((g_x)_i)$; surface forcing $g_f = ((g_f)_i)$; and open boundary conditions $g_b = ((g_b)_i)$.

The contribution of each observation platform to the total transport increment $\Delta J_{37N}$ during each 4D-Var analysis cycle of WC10 is shown in Fig. 9a. For reference, the total number of in situ observations from different platforms during every cycle is shown in Fig. 9c. In addition, during a typical cycle, $\sim 10^5$ satellite SST observations are assimilated, so satellite data form the lion’s share of all available observations. While on average satellite SST is the dominant observation platform controlling $\Delta J_{37N}$, it is also noteworthy that observations from further afield exert significant influence as well. SST observations offshore are important as well. SST dominates the rms average impact over all cycles; although, collectively, in situ hydrographic observations and satellite SSH exert approximately the same impact as SST. The contributions of each observation platform to $\Delta J_{37N}$ associated with the 4D-Var increments to $\delta x(t_0), \delta f(t) \text{ and } \delta b(t)$ of Fig. 4a are qualitatively similar to Fig. 9a.

Fig. 10 shows the rms contribution of data from each observation location from different platforms to the total transport increment $\Delta J_{37N}$ averaged over all WC10 assimilation cycles during the July 2002–December 2004 period. The platforms shown are which Fig. 9a indicates have a consistently large impact on $\Delta J_{37N}$, namely SST, SSH and salinity observations from Argo floats and CTDs. Fig. 10a shows that coastal SSH poleward of 45°N, on average, exerts a large impact on 37°N transport increments, although SSH observations offshore are important as well. Fig. 10b also reveals the relative impact of a single satellite observation and a single hydrographic cast. While each satellite datum location is sampled many times during the 2002–2004 period, an Argo float seldom (if at all) occupies the same location more
than once. A comparison of the color bars associated with the various panels in Fig. 10 reveals that a single vertical profile of $S$ typically exerts considerably more influence on $D_{J37N}$ than any individual satellite observation point. Therefore, despite the relatively small number of subsurface in situ observations compared to the satellite data (Fig. 9c), in situ observations yield a larger impact per datum.

5.2. 500 m isobath transport analysis

A time series of the total transport increment $\Delta J_{500m}$ is shown in Fig. 9b. SST observations generally dominate in this case also. Fig. 9b shows that on average, the collective impacts of in situ observations and SSH on $D_{J500m}$ are as important as SST. The rms impact of data from each observation location on $D_{J500m}$ is shown in Fig. 11 for SSH and SST. Fig. 11a is quantitatively similar to Fig. 10a although the impacts of SSH on $D_{J500m}$ are generally smaller than the impact on $D_{J37N}$. The coastal impacts of SST on $D_{J500m}$ in Fig. 11b are less extensive than those in Fig. 10b for $D_{J37N}$, while the impacts of $S$ observations from Argo floats and CTDs on $D_{J500m}$ are qualitatively similar to those of $D_{J37N}$ (not shown).

5.3. Forecast cycle impacts

During any forecast cycle, the squared forecast error difference $\delta e$ given by (8) can also be expressed as:

\[
\delta e = (k_a - k_b)^{-2} d^T J_{\delta x} J_{\delta x} \hat{M}_x \left( \left( J_f^0 - J_x^0 \right) \sum_{k=k_q}^{k_h} \left( M_{i,k} \right)_{kk} h_k \right)
\]

\[
+ \left( J_f^0 - J_x^0 \right) \sum_{k=k_q}^{k_h} \left( M_{i,k} \right)_{kk} h_k \]

(12)

where $M_{i,k}$ represents the integration of the adjoint model backwards in time over the assimilation cycle that spans $[t_0^0 + 7, k t_0^0]$, and linearized about the background circulation $\hat{x}(t)$ for that cycle. As defined earlier ($M_{i,k} = \hat{M}_x \left( t_0^0 + 7, k t_0^0 \right) = \hat{M}(k_2 \Delta t, k_2 \Delta t)$), integrations of ADROMS terminate at time $t_0^0 + 7 = k_2 \Delta t$. The observation impacts on $\delta e_{37N}$ and $\delta e_{500m}$ during each forecast cycle are shown in Fig. 12, and the relative contributions of the individual observing platforms are similar to those of the analysis cycle impacts discussed in Sections 5.1 and 5.2.

5.4. The dynamics of observation impacts

The observation impacts of Sections 5.1, 5.2, 5.3 are the result of several factors, some dynamical and some statistical. Advection and wave propagation will both influence the spatial dependencies of the impacts in Figs. 10 and 11, although the distance over which information can propagate via these processes differs substantially. In the case of horizontal advection, the speed of the California Current is $\approx 0.1$ m s$^{-1}$ (Hickey, 1998), while in the case of waves, the...
first baroclinic wave mode phase speed is \( \sim 2 \text{ m s}^{-1} \) (Chelton et al., 1998) with barotropic wave speeds being two orders of magnitude larger. Therefore it is useful to think of horizons for advection and wave motions that represent the farthest distance over which information from the observations can be expected to propagate during an analysis or forecast cycle and at the same time influence \( J_{37N} \) and \( J_{500m} \). For the 7 day intervals considered here, the horizontal advection horizon extends only \( \sim 60 \text{ km} \) from the 37\(^{\circ}\)N and 500 m isobath sections shown in Fig. 1b. The first baroclinic mode wave horizon on the other hand will extend almost all the way to the open boundaries in the case of non-dispersive coastally trapped waves and short inertia-gravity waves, while the barotropic wave horizon will encompass the entire model domain. The coastal wave guides will also act to channel information along the coast which is quite evident in Figs. 10 and 11.

In addition to dynamical influences, the prior error covariances \( D \) imposed on 4D-Var will act to spread information spatially, \( \sim 100 \text{ km} \) in the case of the initial conditions, and \( \sim 600 \text{ km} \) in the case of the surface forcing. The multivariate balance operator (Part I, Section 5.2) may also yield some non-local influences when the elliptic equation for balanced free surface height increments is used (cf. Eq. (20) of Part I).

While some of the observation impacts are associated with a positive influence of the observations to the ocean circulation analyses, some of the impacts will also be detrimental. The latter may arise from several factors, including erroneous data, model error, (i.e. where the model struggles or is unable to reproduce an observed field value), errors in the forcing, and initialization shocks associated with dynamical imbalances that invariably exist at the beginning of each data assimilation cycle. Some of these effects are evident in the time evolution of the array modes (see Part II, Section 6.3) and representer functions for individual observations (not shown). Therefore continuous monitoring of observation impacts will be useful for identifying suspicious observation platforms as well as areas of poor model performance and likely model error.

### 6. Observation sensitivity

As described in Part I (Section 7.3), the analysis (posterior) control vector \( z \) can be expressed as:

\[
z = z^b + \kappa(d)
\]

(13)
where \( \mathcal{K}(\mathbf{d}) \) represents the entire data assimilation procedure, and is a nonlinear function of the innovation vector \( \mathbf{d} \) by virtue of the conjugate gradient method used to identify the cost function minimum. In addition, \( \mathcal{K}(\mathbf{d}) \equiv \mathbf{Kd} \) and the practical gain matrix \( \mathbf{K} \) is also a function of \( \mathbf{d} \) according to the Lanczos vector formulation of the conjugate gradient method that is employed in ROMS 4D-Var. As described in Part I (Section 4), the first member of the Lanczos vector sequence \( \mathbf{q}_1 = \mathbf{d} / j\mathbf{d}j \) in the case of 4D-PSAS and R4D-Var, while \( \mathbf{q}_1 = \mathbf{G}^T \mathbf{R}^{-1} \mathbf{d} / j\mathbf{G}^T \mathbf{R}^{-1} \mathbf{d}j \) in the case of 4D-Var, and subsequent members of the sequence also depend on \( \mathbf{d} \) according to the Lanczos recursion relation (Part I, Eq. (15)). In Section 5 we explored the impact of each observation on the alongshore and cross-shore transport, \( \mathcal{J} \). However, the sensitivity of \( \mathcal{J} \) to variations \( \mathbf{y}^e \) in the observations is of considerable interest. A change \( \mathbf{y}^e \) in the observation vector \( \mathbf{y}^o \) leads to a change \( \mathbf{d} = \mathbf{K}(\mathbf{d} + \mathbf{y}^e) - \mathbf{K}(\mathbf{d}) \approx (\partial \mathbf{K} / \partial \mathbf{y}^e) \mathbf{y}^e \) in the analysis, where \( (\partial \mathbf{K} / \partial \mathbf{y}^e) \) represents the tangent linearization of 4D-Var. The corresponding change in the scalar function \( \mathcal{J} \) is given by

\[
\delta \mathcal{J} \simeq (\mathbf{dx}^e)^T (\partial \mathcal{J} / \partial \mathbf{x}) \bigg|_{\mathbf{x}^e},
\]

where \( \mathbf{dx}^e \) is the change in the state-vector increment associated with \( \mathbf{d} \), and \( \mathcal{M}_e \) is the tangent linear model linearized about \( \mathbf{x}_e(t; t_0) \) in the case of I4D-Var and 4D-PSAS, and \( \mathbf{x}_e(t) \) in the case of R4D-Var. More specifically we have:

\[
\delta \mathcal{J} \simeq (\mathbf{dx}^e)^T (\partial \mathcal{J} / \partial \mathbf{x}) \bigg|_{\mathbf{x}^e} = \delta \mathcal{J}^T \mathcal{M}_e^T (t) \mathcal{J} (t) \bigg|_{\mathbf{x}_e} \quad \delta \mathcal{J}^T (\partial \mathcal{K} / \partial \mathbf{y}^e)^T \mathcal{M}_e^T (t) \mathcal{J} (t) \bigg|_{\mathbf{x}_e},
\]

where \( (\partial \mathbf{K} / \partial \mathbf{y}^e)^T \) represents the adjoint of the entire tangent linear 4D-Var system. For the alongshore or cross-shore transport introduced in Section 4, Eq. (15) becomes:

\[
\delta \mathcal{J} \simeq (k_2 - k_1)^{-1} \delta \mathbf{y}^e^T (\partial \mathcal{K} / \partial \mathbf{y}^e)^T \sum_{j=k_1}^{k_2} (\mathcal{M}_j^T) \mathbf{h}_s.
\]
The relationship between the observation impact calculations of Section 5 and the sensitivity to the values of the observations can be appreciated by considering the special situation $\Delta y^o = d$, in which case $K(d + \Delta y^o) = K(d)$. If $K(d)$ is weakly nonlinear, then $K(2d) \approx 2K(d)$ and $\delta z = (\partial K/\partial y^o)\Delta y^o \approx K(d) \equiv Kd$. Substituting $\Delta y^o (\partial K/\partial y^o) \approx K(d)$ in (16) yields, in the case of R4D-Var where $M_d = M_a$, the observation impact Eq. (9). Therefore, in the case $\Delta y^o = d$ the observation sensitivity given by (16) yields the 4D-Var transport increments $\delta J = \Delta J(x^o) - J(x^o)$. We will demonstrate the validity of this result below.

Fig. 13 illustrates schematically the difference between the observation sensitivity and the observation impacts of Section 5. For a given set of observations $y^o$, the observation impact of (9) quantifies the contribution of each observation $y^i$ to the resulting increment $\Delta J$. Conversely, if the values of the observations were to change by $\Delta y^o$, then the observation sensitivity (16) reveals how each $\delta J^i$ contributes to the corresponding change $\delta J$ in $J$.

6.1. Analysis cycle sensitivity

6.1.1. Sensitivity vs. impact

While (9) and (16) will yield approximately the same value for $\Delta J(t)$ and $\delta J(t)$ when $K(d)$ is weakly nonlinear, the contribution of each observation platform to the dot-products in the two equations will in general be quite different. This is illustrated in Fig. 14 for 37N transport, $J_{37N}$, introduced in Section 4, for a representative 7 day R4D-Var assimilation cycle spanning the period 29 March–3 April, 2003 using WCI1. Fig. 14a shows the total number of observations from each observing platform that were assimilated into the model during this cycle. The contribution of the observations from each platform to the total transport increment $\Delta J_{37N}$ computed from the observation impact (9) is shown in Fig. 14b. While most of the observations are in the form of satellite SST measurements (Fig. 14a), SST accounts for only about 20% of the total transport increment. The remaining 80% is distributed amongst the other observation platforms, with salinity observations from CTDs contributing the largest fraction. In this example, the transport increments due to SSH and Argo observations are in the opposite sense to those of SST and CTDs.

Fig. 14c shows $\delta J_{37N}$ according to the observation sensitivity (16), and a comparison of Fig. 14b and c shows that the observation sensitivity of (16) and observation impact of (9) do indeed yield the same total transport increment $\Delta J_{37N}$ confirming the weakly nonlinear nature of $K(d)$ in this case. However, Fig. 14b and c also reveal that the contribution of each observation platform to $\Delta J_{37N}$ and $\delta J_{37N}$ is very different. While the observation impact calculation of Fig. 14b indicates that Argo salinity observations contribute most to the increment $\Delta J_{37N}$, Fig. 14c reveals that $\delta J_{37N}$ is actually most sensitive to variations in the SSH observations.

To understand these differences, consider again the observation impact calculation of (9). The partial sums in Fig. 14b represent the actual contribution of each observation to $\Delta J_{37N}$ for the specific data assimilation cycle considered (cf. Fig. 13). Conversely, $\delta J_{37N}$ computed using (16) represents the change in transport that would occur if the observation vector $y^o$ undergoes a change $\Delta y^o = d$ (cf. Fig. 13). Clearly the meaning and interpretation of (9) and (16) is very different and despite being numerically the same, there is no requirement for the partial sums representing the contribution of each observation platform to $\Delta J_{37N}$ and $\delta J_{37N}$ to be the same, except when either (a) the assimilation procedure is truly linear (Trémolet, 2008), or (b) in the case when the number of inner-loops $m = N_{obs}$, so that $K = \partial K/\partial y^o = K$, the true gain matrix.

6.1.2. Observing system experiments (OSEs)

The observation sensitivity Eq. (15) can be used to determine how $J$ will change due to the degradation or failure of an observation platform or if some of the data are corrupted and unusable. Another possibility of course is to recompute the 4D-Var analyses withholding the observations in question, the procedure usually employed in observing system experiments (OSEs). However, this is a costly process, and the same information may be directly available from the observation impact or observation sensitivity calculations.

One might expect from the observation impact calculations of Fig. 14b that if, say, the altimeter were to fail during the 4D-Var cycle in question, the transport would decrease by ~0.1 Sv. However, this will not necessarily be the case since withholding all of the SSH observations will fundamentally alter $K$ and the circulation increment, and there is no guarantee that the contributions of the remaining observations to the dot-product for $\Delta J$ given by (9) will be the same as they were before. Alternatively, the observation sensitivity (15) could be used to predict the change

Fig. 13. A schematic illustrating the fundamental difference between the observation impact and observation sensitivity calculations. Each curve represents the evolution of the ocean state vector $x$ in time based on the either the prior or posterior control vector. Individual observations, $y^o_i$, at various times are shown as plusses (+) while perturbed observations, $y^{o,i} + \Delta y^{o,i}$, are indicated by filled circles (•). The value of the functional $J$ computed from each circulation estimate is indicated to the right of the figure, $J_s$ in the case of the prior and $J_a$ in the case of the posterior. In the case of the observation impact, the actual contribution of each observation, $y^o_i$, to the change $\Delta J$ (blue curve vs. black curve) due to data assimilation is revealed. Conversely, the observation sensitivity quantifies the change $\delta J$ that will occur in $J_a$ (red curve vs. blue curve) as a result of perturbations in the observations, $\Delta y^o$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
expected in $J$ arising from changes $\delta y_i = -d_i$ in some of the observations. This would cause the innovations associated with the affected observations to vanish, and is tantamount to perfect agreement between the model background and the affected observations. According to Fig. 14c, a change $\delta y_i = -d_i$ in all of the SSH observations would yield an increase in alongshore transport $\approx 0.6\, \text{Sv}$, some six times larger and in the opposite sense to the change predicted by the observation impact of Fig. 14b.

Observation sensitivity calculations require $(\partial J/\partial y)^T$, however at the present time the adjoint of 4D-Var is only available in ROMS for the dual formulation. As shown in Part II (Section 3.1) the dual formulation is considerably less efficient than the primal form, in which case the period July 2002–December 2004 (comprised of 123 assimilation cycles) represents a considerable computational challenge for WC10. Therefore we will demonstrate the utility of observation sensitivity using a coarser resolution model with 1 outer-loop and 50 inner-loops spanning 7-day assimilation cycles. As shown in Part II (Fig. 2b and Fig. 4) this is sufficient to guarantee a significant level of convergence of $J$ towards its minimum value using 4D-Var at this resolution. Fig. 2 also shows the ratio of the final and initial values of $J$ for the 4D-Var sequence using WC30 where an order of magnitude reduction in $J$ during each cycle is typical.

Using the WC30 4D-Var sequence, the changes in $J$ predicted by the observation impact and observation sensitivity calculations were compared with direct calculations in which observations were withheld during each 4D-Var cycle. However, in the interest of space, we will confine our attention to the alongshore transport only. Fig. 15a shows a time series of the prior transport $J_{37N}$ in WC30 which is qualitatively similar to that of WC10 shown in Fig. 3a. The transport increments $\Delta J_{37N}$ and the contribution of each observation platform to $\Delta J_{37N}$ computed from the observation sensitivity (16) assuming a perturbation in the observations $\delta y = d$. There were no XBT or TOPP data available during this 7 day period. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
There is considerable variability from cycle-to-cycle, and during some cycles subsurface observations from CTDs, Argo floats, and XBTs are more influential than the satellite observations. Fig. 15c, on the other hand, shows $\Delta J_{37N}$ based on the observation sensitivities calculated using (16) for the case $dy_o = d$. While $\Delta J_{37N}$ in Fig. 15b and $\Delta J_{37N}$ from (16) are indistinguishable during each R4D-Var cycle as shown in Fig. 15d, the sensitivity of $\Delta J_{37N}$ suggested by (16) for perturbations $dy_o = d$ in the observations (Fig. 15c) indicates that $J_{37N}$ will be influenced considerably by any changes in the SSH coverage. An inspection of the geographical variations in the observation sensitivities reveals that $J_{37N}$ is most sensitive to variations in the observations in the vicinity of the 37°N section (not shown).

Predictions of the change $\Delta J_{37N}^p$ in $J_{37N}$ expected when observations are withheld are shown in Fig. 16 based on the observation impacts and observation sensitivities of Fig. 15b and c. In the case of the observation sensitivity calculations, $dy_o = d$ for the observations that were withheld. Two cases are shown; one in which all Argo observations were withheld (Fig. 16a), and another in which all SSH observations were withheld (Fig. 16b). Also shown in Fig. 16 are time series of the actual changes $\Delta J_{37N}$ that occurred when each R4D-Var analysis was repeated in the absence of Argo floats or SSH observations. It is important to note that Fig. 16

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3 This is somewhat in contrast to the situation in WC10 shown in Fig. 9a where SST observations exert the largest impact during most cycles. The difference between the observation impacts in WC10 and WC30 can be easily understood in terms of the spatial resolution of the satellite product used in the two models. The gridded SSH observations used in both cases have a spatial resolution of $\sim 1/3'$. The blended SST product, however, has a resolution of 10 km which is higher than the resolution of WC30. As described in Section 3 the procedure of forming super observations averages the satellite SST to provide a single observation per model grid cell, meaning that there are $\sim 10$ times more SST observations assimilated into WC10 than in WC30.
shows the case where each R4D-Var analysis cycle was considered independently. Therefore, in the case of analysis cycle \( j \), all observations were assimilated during all of the preceding \((j - 1)\) analysis cycles, and observations were withheld only during cycle \( j \). Fig. 16a indicates that in general, the agreement between \( \delta J_{t_{37N}} \) and \( \delta J_{p_{37N}} \) predicted by the observation sensitivity given by (16) is excellent in the case when Argo float observations are withheld. The agreement between \( \delta J_{t_{37N}} \) and \( \delta J_{p_{37N}} \) from (16) is also generally very good when all SSH observations are withheld (Fig. 16b), although in this case the discrepancies are somewhat larger. However, in both cases the observation impacts given by (9) are a very poor predictor of \( \delta J_{t_{37N}} \).

The results of Fig. 16 indicate that, the observation sensitivity given by (16) provides a reliable means of estimating the impact on \( J \) of changes in the observations or observation array on a cycle-by-cycle basis without the need to recompute the 4D-Var analysis.

As described in (Part I, Section 3.2.3), the dual formulation of 4D-Var is equivalent to solving the original linear system with the elements of \( d \) corresponding to the withheld observations set to zero. Clearly the dimension of the linear equations that are solved in the two cases will be different, but if the dimension of the two systems is similar (i.e. if only a small percentage of the observations are withheld) then we would expect similar solutions for the elements of \( w \) that correspond to the observations that are common in both cases. This is certainly the case, for example, in Fig. 16a where the Argo observations are withheld. Even in Fig. 16b where all SSH observations are withheld, a case where there is a significant change in the dimension of \((GDG^T + R)\), direct computations of dual 4D-Var and observation sensitivity based on \( \partial K / \partial y \) agree very well. However, in general we anticipate that the agreement between direct dual 4D-Var computations and the predictions of \( \partial K / \partial y \) will deteriorate as the number of observations withheld continually increases.

The calculations presented here were performed using only a single outer-loop. For the case of multiple outer-loops, the second derivative of NLROMS is required but is not available. However, Trémolet (2008) argues that using the nonlinear model solution \( x \) from the first outer-loop yields a good approximation for observation sensitivity calculations in the case of multiple outer-loops.

In the foregoing analysis, the impact of withholding observations on the transport was examined by considering each assimilation cycle of the sequence independently, meaning that the observations that were withheld impact only the cycle in question.
However, it is more usual during OSEs to repeat the entire assimilation sequence so that each new analysis with observations withheld becomes the background for the next cycle. Thus the impact of withholding observations propagates from one cycle to the next. Consider then two sequences of ROMS CCS 4D-Var analyses, a control in which all observations are assimilated, $x^0$, and an OSE in which some of the observations are withheld, $x^1$. Suppose also that the background initial condition for the first cycle, $j = 1$, is the same for both the control and OSE sequences, and that the background surface forcing $f^i(t)$ (i.e. from COAMPS) and background boundary conditions $b^j(t)$ (i.e. from ECCO) are the same for all members of both sequences. At the end of the first cycle, the analyses from the two sequences will be different, and this difference will propagate to the next member of the sequence, $j = 2$, via the background initial conditions. Therefore, as each sequence proceeds, $x^0$ and $x^1$ will become decorrelated until eventually the variance of $\Delta x^j_t = x^j_t - x^0_t$ is equal to the climatological variance of either sequence. For the mesoscale circulation environments considered here, experience reveals that this can happen after only a few months. It is of interest then to consider the utility of observation sensitivity in predicting the relative changes in the function $J$ arising from the control and OSE sequence of analyses. Specifically, if $\Delta J^j_t = J^j_t(x^j_t) - J^j_t(x^0_t)$ and $\Delta J^j_{o,e} = J^j_t(x^j_t) - J^j_t(x^0_t)$ are the corresponding sequences of $37^\circ$N transport increments of the control and OSE, then consider the sequence of differences $\Delta J^j_{o,e} = \Delta J^j_t - \Delta J^j_{o,e}$. The mean and standard deviation of $\Delta J^j_{o,e}$ over all cycles are therefore measures of the average impact (relative to the control) of withholding the observations during the OSE on the transport increments. Fig. 16c shows a time series of $\Delta J^j_{o,e}$ for an OSE during which all SSH observations were withheld. Also shown in Fig. 16c is the time series of predictions $\delta J^j_{o,e} = \delta J^j_{o,e}$ based on the observation sensitivity (16) with $\delta^j_y = -d$ for all SSH observations. The level of agreement is very good, and the correlation between the two time series is 0.77. The mean and standard deviation of $\Delta J^j_{o,e}$ and $\delta J^j_{o,e}$ are $-0.28 \pm 0.81$ Sv and $-0.26 \pm 0.65$ Sv respectively. On the other hand, a similar analysis for an OSE during which all Argo float observations were withheld shows almost no correlation between $\Delta J^j_{o,e}$ and $\delta J^j_{o,e}$ based on (16) (not shown). The reason why the SSH case is successful and the Argo case is not is that both cases are not understood by the observation number of data, the data distribution, and the observation impact for each data type. In the case of SSH, recall that the observations used here are in the form of the gridded Aviso product. Therefore during the OSE, many observations are withheld and they are spatially coherent. As shown in Fig. 10a, the SSH observations from primarily two areas impact $J_{37^\circ}$, namely observations along the coast and observations in deep water and the patterns of impact are spatially coherent over large scales. Therefore, irrespective of the background circulation, $x^j(t)$, used during 4D-Var, a given set of SSH observations will yield a similar change $\Delta J^j_{o,e}$ in $J_{37^\circ}$, and this change is captured by (16) for any background. Conversely, in the case of Argo floats, the observations are few in number and randomly distributed in space, so their impact on $J_{37^\circ}$ during any 4D-Var cycle (cf. Fig. 10c) will be dependent on the background circulation. Accordingly, since the sequences of background observations $x^j(t)$ and $x^0(t)$ decorrelate over time, so too will the sequences of $\Delta J^j_t$ and $\Delta J^j_{o,e}$ for the Argo float OSE.

The observation sensitivity (16) based on the adjoint of the entire 4D-Var system is therefore not only a useful tool for OSEs when each cycle is considered independently, but is also a reliable predictor of observation impacts during an OSE sequence when the observations considered are spatially coherent, such as in the case of satellite observations or rapid repeat samples from, say, gliders or AUVs.

6.2. Forecast cycle sensitivity

The sensitivity of the forecast errors in $J_{37^\circ}$ to changes in each observation can also be assessed using the appropriate form of (15) (see Part I, Section 7.3). In Section 5.3 we examined the impact of each observation platform on the difference in $J_{37^\circ}$ forecast error between 7 and 14 day forecasts that verify over the same interval (cf. Fig. 5) using WC10. The same calculations were performed using WC30 where in this case $J_{37^\circ}$ represents the transport averaged over the last 48 h of the forecast. A first-order Taylor approximation $^4$ for $\delta e$ resulting from a change $\delta y^j$ in the observations during the preceding analysis cycle yields:

$$
\delta e = 2(k_4 - k_3)^{-1} \left( J^j_t - J^o_t \right) \delta y^j / \partial J^j_t / \partial J^o_t \left[ \mathbf{M}^j_t \mathbf{M}^o_t \right]_{0} \times \sum_{k=4} \left( \mathbf{M}^j_t \right)_{k} \mathbf{h}_k
$$

where all terms are as defined in Section 5. Fig. 17a shows time series of $\delta e$ computed from (17) with $\delta y^j = \mathbf{d}$ and from the first-order equivalent of the observation impact (8); $\delta e$ is indistinguishable in both cases again confirming the weakly nonlinear nature of $k_4(d)$. The contributions of each observation platform to $\delta e$ based on observation sensitivity and observation impact are shown in Fig. 17b and c respectively, and in both cases SSH plays a dominant role.

The expected change in $e_{37^\circ}$ due to withholding observations predicted by the observation impacts and observation sensitivities of Fig. 17 are shown in Fig. 18 for the case where all Argo floats or all SSH observations are withheld. The actual change in $e_{37^\circ}$ computed directly from forecasts initialized from R4D-Var analyses in which all observations from each platform were withheld is also shown. In this case observation sensitivity is a very good predictor of the change in $e_{37^\circ}$ when Argo data are withheld (Fig. 18a). The observation impact predictions are also quite good in this case during some cycles, but in general the agreement with the directly computed change is quite poor. In the case where SSH observations are not assimilated, observation sensitivity and observation impact predictions are very similar, and both agree reasonably well with the direct calculations, although the amplitude of the change in $e_{37^\circ}$ is often underpredicted. Therefore, we conclude that overall, it appears that observation sensitivity is a robust predictor for OSEs during both analysis and forecast cycles.

6.3. Uncertainty analysis

The adjoint of 4D-Var, $(\partial J^j_t / \partial y^j)^\dagger$, is also a very efficient tool for quantifying the uncertainty of the resulting circulation estimates arising from uncertainties in the observations. According to (16), the change in $37^\circ$N transport due to a change in the observations $\delta y^j$ is given by $\delta J_{37^\circ} = \delta y^j R g$, where $g = (k_2 - k_1)^{-1} \left( \partial J^j_t / \partial y^j \right)^\dagger \sum_{k=1} (\mathbf{M}^j_t)^k (\mathbf{B}^j_{37^\circ} k) = \partial J^j_t / \partial y^j \mathbf{R} g$. The uncertainty in the observations is described by the observation error covariance matrix $\mathbf{R}$ which is a precise statement about our prior assumptions regarding random instrument errors and errors of representativeness. In light of this, the observation vector can be expressed as $y^j - \delta y^j$ where the $\delta y^j$ is a sequence of different realizations of random observation errors drawn from the normal distribution with covariance $\mathbf{R}$ so that $E(\delta y^j \delta y^j)^\dagger = \mathbf{R}$, where $E$ is the expectation operator. The variance in the uncertainty of the resulting analysis of $J_{37^\circ}$ due to uncertainties $\delta y^j$ in the observations is then given by $\sigma_J^2 = E(\Delta J_{37^\circ}^2) = E(\mathbf{g}^\dagger \delta y^j \delta y^j / \partial J_{37^\circ} / \partial y^j \mathbf{g}) = \mathbf{g}^\dagger \mathbf{R} \mathbf{g}$. Fig. 19 shows a time series of the standard deviation $\sigma_J$ for the

$^4$ A first-order approximation is adequate in WC30 because of the relatively coarse horizontal resolution compared to WC10.
Fig. 17. (a) A time series of the difference between the 7 and 14 day WC30 forecast error $\delta e_{37N}$ based on observation impact (red curve) and observation sensitivity calculations (blue curve) for $d = d_{yo} = 0$, where the two time series are indistinguishable. (b) Time series of the contribution to $\delta e_{37N}$ for each observation platform based on observation sensitivity calculations. The rms contribution of each observation platform averaged over all cycles is also indicated. (c) Same as (b) except based on the observation impact calculations. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 18. Time series (green curves) of the change in $e_{37N}$ computed directly from the background and analysis circulation estimates of each 7-day R4D-Var cycle in WC30 when (a) all Argo float observations are withheld, and (b) all satellite SSH observations are withheld. Also shown are time series (red curves) of the predicted change in $e_{37N}$ based on observation sensitivity calculations with $d = d_{yo} = 0$, for either all Argo float or SSH observations. Time series of the change in $e_{37N}$ predicted by observation impact calculations are shown by the black curve. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
WC30 sequence of R4D-Var cycles described earlier, and indicates that the uncertainty in 37°N transport associated with instrument error and errors of representativeness is \( \pm 0.12 \) Sv. Since the elements of \( g \) are unambiguously associated with each individual observation, the contribution of the different observation platforms to the variance \( \sigma^2_r \) can also be evaluated as shown in Fig. 19. Fig. 19 reveals that, on average, two thirds of the expected variance in the uncertainty in \( J_{37^n} \) is associated with SSH observations, and that most of the remaining third is associated with uncertainty in SST. However, during some cycles the uncertainty associated with in situ observations is a significant contributor to \( \sigma^2_r \) also. While we have considered here only uncertainties in \( J_{37^n} \) arising from \emph{a priori} errors in the observations, uncertainties in the background initial conditions, surface forcing, boundary conditions and model dynamics will also contribute to the expected errors in the analyses. The adjoint of 4D-Var can also be used to quantify the contributions of these components of error to the expected uncertainty in \( J_{37^n} \) as shown in Moore et al. (submitted for publication).

7. Summary and conclusions

Sequential application of ROMS 4D-Var to the California Current System demonstrates that data assimilation yields substantial changes in the background ocean circulation estimates. The contribution of the different components of the increment control vector and each observation platform to these changes can be assigned using methods established in numerical weather prediction to quantify observation impacts. In addition, the sensitivity of the circulation estimates to changes in the observations or observing network can also be assessed using the adjoint of the 4D-Var system. Both observation impact and observation sensitivity calculations rely on the property of adjoint operators to identify the part of state-space that is activated by the observations. To our knowledge, this paper describes the first oceanographic application of these methods which constitute important and powerful diagnostic tools that are available as part of the ROMS 4D-Var system.

In this study we focus our attention on measurements of the alongshore and cross-shore transport that are strongly controlled by seasonal changes in coastal upwelling. Despite the complex and nonlinear nature of the CCS circulation, the tangent linear assumption employed in all of the calculations is valid for periods of \( \sim 7 \) days, and faithfully reproduces transport changes in the nonlinear model. Here we have explored the observation impact and observation sensitivity during 4D-Var analysis cycles and the subsequent forecast cycles initialized from the circulation estimates of 4D-Var.

The primary purpose of this paper is to demonstrate the power and utility of the ROMS observation impact and observation sensitivity capabilities. However, despite the regional focus of the calculations presented here, many of our conclusions are likely to be applicable to the broader CCS circulation, and to perhaps other eastern boundary currents. For instance, while the relative impact of uncertainties in the initial conditions, surface forcing, and boundary conditions on circulation estimates has remained an open question for some time, results presented here demonstrate that weekly analyses of the alongshore transport at the heart of a coastal upwelling region are influenced primarily by uncertainties in the initial conditions and surface forcing. There is, however, considerable variability from one assimilation cycle to the next, with the initial condition increments dominating during some cycles, and the forcing increments dominating during others. On the other hand, cross-shore transport associated with wind-induced upwelling is generally influenced most by uncertainties in the surface forcing. Forecasts initialized from each 4D-Var analysis, on the other hand, possess only a limited memory of the surface forcing increments that are so critical for the efficacy of the analyses. Instead, much of the forecast error is governed by the initial conditions of the 4D-Var analysis cycle, and much of the information from the forcing increments is rapidly lost, suggesting perhaps that the intrinsic hydrodynamic properties of the circulation (such as instabilities) are the primary controlling factor.

Perhaps surprisingly, uncertainties in the open boundary conditions exert a relatively small influence on the analysis coastal transport estimates. However, the relatively short 7 day analysis cycles considered here may not allow sufficient time for baroclinic effects to reach the coast from the boundaries. In addition, the presence of a sponge layer at the open boundaries may act to suppress some of the boundary influences on the interior circulation.

While observations of the CCS are available from a range of platforms and products, their impact on the coastal transport depends on the horizontal resolution of the model. For convenience a gridded AVISO SST product was used here with a spatial resolution that closely matches the resolution of WC30. On the other hand, the resolution of the blended satellite SST product must be decimated via the formation of super observations before it can be assimilated into WC30. As a result a similar number of SST and SSH observations were assimilated into WC30 during a typical 4D-Var cycle, and on average SSH has the largest impact on coastal transport in WC30 during both the analysis and forecast cycles. Conversely, in WC10 the resolution of the SST observations closely matches that of the model grid, so very few super observations need to be formed, meaning that there are an order of magnitude more observations of SST than SSH that can be assimilated into WC10. In this case, SST observations most often exert the largest influence on the coastal transport during both the analysis and forecast cycle. However, in both models when subsurface observations from other platforms are available, they often exert considerable influence that collectively is comparable to that of satellite data. Therefore an important finding of the observation impact calculations presented here is that they clearly demonstrate the important
influence of subsurface observations on the analysis and forecast circulations, even though these observations are typically few in number compared to satellite observations. The impact of SSH observations close to the coast also highlights the need for reliable altimeter measurements in these regions where existing observations are known to be deficient (Saraceno et al., 2008).

While it is mainly observations near the coast that have the largest impact on coastal transport, observations further offshore can also be important. The impact of remote observations on coastal transports can be understood in terms of wave dynamics and changes in large-scale pressure gradients, while the more local influences are most likely associated with horizontal advection. In addition, spatial variations in the observation impacts reveal clear signatures associated with coastally trapped waves. On the other hand, the coastal impacts of observations in deep water can be attributed to changes in the large-scale pressure gradient and to fast barotropic waves and/or short baroclinic inertia-gravity waves that carry information to the coast. This raises questions about the dynamical significance of the remotely excited waves as vehicles for transmitting information within the model domain. While some of these waves will be associated with legitimate dynamical adjustment processes in response to the assimilation of observations, others will be the result of spurious initialization shocks resulting from the inevitable dynamical imbalances that are present in the initial conditions.

Initialization shock remains a perpetual issue in data assimilation (Dailey, 1991), but is not often addressed in the oceanographic literature. Our experience here, however, indicates that observation impact analysis could be used to identify and isolate observations that contribute most to initialization shocks. For example, choosing a basin integral of the squared vertical velocity might be a convenient and illuminating approach for identifying those observations that are prone to excite large amplitude inertia-gravity waves. A subsequent reanalysis 4D-Var cycle with the offending observations withheld may then yield a superior quality circulation estimate.

In contrast to the observation impact calculations which quantify the contribution of each observation to functions \( J \) of the state-vector during an analysis or forecast cycle, the observation sensitivity calculations reveal the change that will occur in \( J \) if the observations change. Observation sensitivity has tremendous utility since we find that when each analysis-forecast cycle is considered independently, the adjoint of 4D-Var can be used to reliably predict the changes that will occur in \( J \) in the event of a platform failure or a change in the observation array. In addition, observation sensitivity can reliably predict the change in \( J \) during an observation system experiment (OSE) sequence of 4D-Var analyses when the observations withheld yield consistent, spatially coherent circulation increments, irrespective of the background circulation. While the adjoint of the 4D-Var system requires the same computational effort as 4D-Var, an observation sensitivity calculation need only be performed once for a given \( J \) making it a computationally efficient tool for OSEs which traditionally require 4D-Var to be rerun for each change in the observation array. Observation sensitivity is therefore a valuable complement to conventional OSEs since the adjoint of 4D-Var provides additional information about circulation uncertainty and sensitivity associated with the observations.

It is important to note that the outcome of the observation impact and observation sensitivity calculations presented here will depend intimately on the prior hypotheses embodied in \( D \) and \( R \). Also, as demonstrated in Part II (Section 6.2) more than 90% of the observations assimilated into ROMS CCS contain redundant information about the circulation on the scales resolved by the model. This level of redundancy is most likely associated with the over abundance of satellite SST observations that are assimilated into the model. Given the large impact of SST on the coastal circulation described by the alongshore and cross-shore transport, it might be prudent to decimate (in space and time) the SST observations before assimilation to reduce the level of redundancy, thereby lowering the relative impact of the SST observations, and allowing the in situ observations to exert more of an influence on the coastal circulation estimates. The use of raw along-track data in the case of SSH and data from individual sensors in the case of SST (as opposed to a blended product) is one obvious approach. Finally we note that the adjoint of 4D-Var has tremendous utility beyond the observation sensitivity calculations presented here. For example, in Moore et al. (submitted for publication) we demonstrate how the adjoint of 4D-Var can be used to compute the expected analysis and forecast errors of linear functions of the state-vector, and provide information about the predictability of the circulation. In addition, the 4D-Var adjoint can be used to efficiently explore the sensitivity of 4D-Var circulation estimates to the many system parameters, such as the \textit{a priori} standard deviations and correlation lengths used to model \( D \) and \( R \). We can also envisage using the adjoint of 4D-Var to optimize the performance of each data assimilation system.

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