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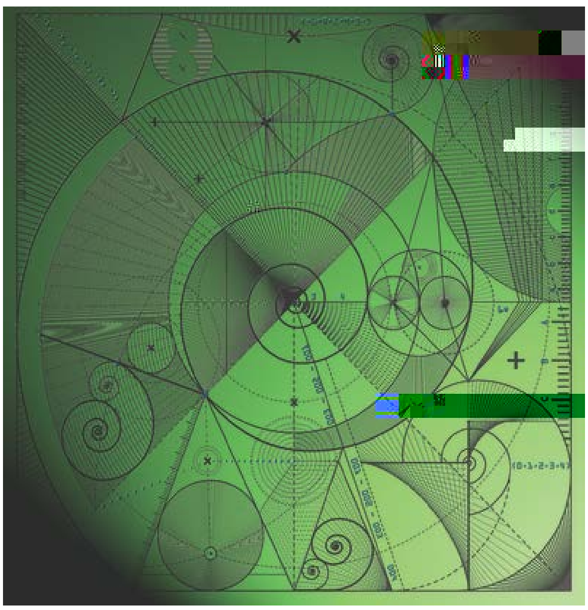

Exploring strategies for coupled 4D-Var data assimilation using an idealised atmosphere-ocean model

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Abstract

Coupled data assimilation o ers a long list of potential bene ts, including improved use of near-surface observations, reduction of initialisation shocks in coupled forecasts and generation of a consistent system state for the initialisation of coupled forecasts across all timescales. Strongly coupled data assimilation presents a signi cant challenge and so several operational centres are developing weakly coupled assimilation systems as a rst step. In this paper we provide a comprehensive description of the di erent coupled assimilation methodologies in the context of four dimensional variational assimilation (4D-Var) and use an idealised framework to assess the expected bene ts of moving towards coupled data assimilation.

We implement an incremental 4D-Var system within an idealised single column atmosphere-ocean model. The system has the capability to run both strongly and weakly coupled assimilations as well as uncoupled atmosphere or ocean only assimilations, thus allowing a systematic comparison of the di erent strategies for treating the coupled data assimilation problem. We present results from a series of identical twin experiments devised to investigate the behaviour and sensitivities of the di erent approaches. Overall, our study demonstrates that signi cant bene ts may be expected from coupled data assimilation. When compared to uncoupled initialisation, coupled assimilation is able to produce more balanced initial analysis elds, thus reducing initialisation shock and its impact on the subsequent forecast. Single observation experiments demonstrate how coupled assimilation systems are able to pass information between the atmosphere and ocean and therefore use near-surface data to greater e ect. We show that much of this bene t may also be gained from a weakly coupled assimilation system, but that this can be sensitive to the parameters used in the assimilation.

Key words: incremental four dimensional variational data assimilation, single column model, KPP mixed layer model, initialisation, strongly coupled, weakly coupled.

1 Introduction

The successful application of data assimilation techniques to operational numerical weather prediction and ocean forecasting systems, together with increasing availability of near surface observations from new satellite missions, has led to an increased interest in their potential for use in the initialisation of coupled atmosphere-ocean models. To produce reliable predictions across seasonal to decadal time scales we need to simulate the evolution of the atmosphere and ocean coupled together. Coupled models have been used operationally for seasonal and longer range forecasting for a number of years. Typically, the initial conditions for these forecasts are provided by combining analyses from independent (uncoupled) ocean and atmosphere assimilation systems (Balmaseda and Anderson, 2009). This approach ignores interactions between the systems and this inconsistency can cause imbalance such that the initial conditions are far from the natural state of the coupled system. When the coupled forecast is initialised the model adjusts itself towards its preferred climatology; this adjustment can produce rapid shocks at the air-sea interface during the early stages of the forecast, a process referred to as initialisation shock (Balmaseda, 2012). It also means that near-surface data are not fully utilised.

The development of coupled atmosphere-ocean data assimilation systems presents a number of scientific and technical challenges (Murphy et al., 2010; Lawless, 2012) and requires a significant amount of resources to be made possible operationally. Yet such systems offer a long list of potential benefits including improved use of near-surface observations, reduction of initialisation shocks in coupled forecasts, and generation of a consistent system state for the initialisation of coupled forecasts across all timescales. In addition, coupled reanalyses offer the potential for greater understanding and representation of air-sea exchange processes in turn facilitating more accurate prediction of phenomena such as El Niño and the Madden-Julian Oscillation (MJO) in which air-sea interaction plays an important role.

Studies have shown that, in certain regions, the initialisation of coupled models can enhance the skill of decadal predictions for the first 5 or so years of the forecast (Meehl et al. (2014) and references therein). Although it is widely accepted that coupled data assimilation has a central role in improving our ability to generate consistent and accurate initial conditions for coupled atmosphere-ocean forecasting it is still a relatively young area of research. Hence there has so far only been limited amount of work in this field. An assortment of strategies for using observed data to improve coupled model initialisation have been explored with varying degrees of success; these include sea surface temperature (SST) nudging or relaxation (e.g. Keenlyside et al. (2008)), anomaly initialisation/ bias-blind assimilation (e.g. Pierce et al. (2004)), anomaly coupling (Pohlmann et al. (2009)), and variants of the full uncoupled initialisation approach (Balmaseda and Anderson, 2009). Work has mainly been focussed on improving ocean initial conditions with a lack of fully consistent treatment of air-sea feedback mechanisms.

There are groups exploring more comprehensive approaches that aim to produce more dynamically balanced initial ocean-atmosphere states. The Japan Agency for Marine-Earth Science and

Fluid Dynamics Laboratory (GFDL) global fully coupled climate model for the initialisation of seasonal and decadal forecasts. The system is evaluated in a series of twin experiments assimilating atmosphere-only or ocean-only observations but not both together. Although the system shows good skill in reconstructing seasonal and decadal ocean variability and trends it fails to fully realise the potential benefit of surface and near surface observational data.

In this paper we explore some of the fundamental questions in the design of coupled variational data assimilation systems within the context of an idealised one-dimensional (1D) column coupled atmosphere-ocean model. The system is designed to enable the effective exploration of various approaches to performing coupled model data assimilation whilst avoiding many of the issues associated with more complex models and allows us to perform experiments that would not be feasible in operational scale systems. We employ an incremental four dimensional variational data assimilation (4D-Var) scheme (Courtier et al., 1994; Lawless et al., 2005; Lawless, 2013) to reflect the coupled assimilation systems currently being developed at the European Centre for Medium Range Weather Forecasts (ECMWF) and UK Met Office. The problem of variational data assimilation is to find the initial state such that the model forecast best fits the available observations over a given time window, subject to the state remaining close to a given *a priori*, or background, estimate and allowing for the errors in each. This best estimate is known as the *analysis* and should be consistent with both the observations and the system dynamics. The standard 4D-Var problem is formulated as the minimisation of a non-linear weighted least squares cost function; in the incremental approach the non-linear problem is instead approximated by a sequence of linear least squares problems. Rather than search for the initial state directly, we solve in terms of increments with respect to an initial background state; this is done iteratively in a series of linearised inner-loop cost function minimisations and non-linear outer-loop update steps.

Strongly or fully coupled assimilation treats the atmosphere and ocean as a single coherent system, using the coupled model in both the inner- and outer-loops. This approach is able to pass information between the atmosphere and ocean, and therefore enables observations of atmospheric variables to influence the ocean increments and vice versa. This is expected to lead to better use of near-surface observations, such as scatterometer winds and SST, that depend on both the atmosphere and ocean state, and to produce a more physically-balanced analysis. Although there are currently no plans to move towards strongly coupled systems at operational centres, this approach represents the quintessential coupled assimilation system and implementing it in our idealised system allows us to better assess the potential of intermediate, or *weakly coupled*, approaches.

As a first step towards the implementation of operational coupled data assimilation, centres such as the ECMWF and UK Met Office are developing prototype weakly coupled assimilation

We begin, in section 2, with the formulation of the general incremental 4D-Var algorithm and a description of the different approaches to coupled atmosphere-ocean 4D-Var data assimilation. We introduce our coupled 1D model system in section 3. In section 4 we give details of a set of identical twin experiments designed to investigate and compare the behaviour and sensitivities of the different approaches. Results are presented in section 5. A summary and conclusions are given in section 6.

2 Incremental 4D-Var data assimilation

Variational methods form the basis of most operational numerical weather prediction (NWP) data assimilation systems (Gauthier et al., 1999, 2007; Rabier et al., 2000; Rawlins et al., 2007; Huang et al., 2009). Our system has therefore been designed using the incremental 4D-Var approach. In this formulation the solution to the full non-linear 4D-Var minimisation problem is replaced by a sequence of minimisations of linear quadratic cost functions such that the control variable in the minimisation problem is the increment to the current estimate rather than the model state itself. The method was originally developed to overcome the cost and practical difficulties involved in solving the complete non-linear problem directly in large scale systems (Courtier et al., 1994). We choose to employ the incremental 4D-Var formulation for this study as it allows us not only to emulate the methodologies being developed for operational systems, but also to explore the type of benefits that could be gained by moving towards strongly coupled assimilation systems, thereby providing a benchmark for the assessment of weakly coupled assimilation systems. We describe each of the different coupled 4D-Var assimilation strategies in detail in section 2.1. To aid these descriptions, we begin with an outline of the steps of the general incremental 4D-Var algorithm.

Let $x_i^{(k)} \in \mathbb{R}^m$ denote the model state vector, representing the system state at a given time t_i and outer-loop iteration k. Then given the discrete non-linear dynamical system model

$$x_i^{(k)} = \mathcal{M}(t_i, t_0, x_0^{(k)}), \qquad i = 0, \ldots, n, \tag{2.1}$$

a background, or first guess, $x_0^{(0)} = x_0^b \in \mathbb{R}^m$, at t_0, imperfect observations $y_i \in \mathbb{R}^{r_i}$ at times t_i, $i = 0, \ldots, N$, and defining the increment

$$\delta x_i^{(k)} = x_i^{(k+1)} - x_i^{(k)}, \tag{2.2}$$

we solve iteratively as described below (Lawless et al., 2005).
For $k = 1, 2, \ldots$ outer-loops, or until desired convergence is reached:

(i) Run the non-linear model (2.1) to obtain $x_i^{(k)}$ at each time t_i.

(ii) Compute the innovations

$$d_i^{(k)} = y_i - h_i(x_i^{(k)}), \tag{2.3}$$

where $h_i : \mathbb{R}^m \to \mathbb{R}^{r_i}$ is a (generally) non-linear observation operator.

(iii) Minimise the least squares cost function

$$\begin{aligned} J^{(k)}\left[\delta x_0^{(k)}\right] &= \frac{1}{2}\left((x_0^b - x_0^{(k)}) - \delta x_0^{(k)}\right)^T B_0^{-1}\left((x_0^b - x_0^{(k)}) - \delta x_0^{(k)}\right) \\ &\quad + \frac{1}{2}\sum_{i=0}^{n}\left(d_i^{(k)} - H_i\,\delta x_i^{(k)}\right)^T R_i^{-1}\left(d_i^{(k)} - H_i\,\delta x_i^{(k)}\right), \\ &:= J_b^{(k)} + J_o^{(k)}, \end{aligned} \tag{2.4}$$

subject to

$$\delta x_i^{(k)} = \mathbf{M}(t_i, t_0, x^{(k)})\,\delta x_0^{(k)}. \tag{2.5}$$

(iv) Update $x_0^{(k+1)} = x_0^{(k)} + \ x_0^{(k)}$, and return to step (i).

In (2.4) B_0 2 $R^{m \ \ m}$ and R_i

atmosphere (ocean) observations and the inner-loop minimisation (step (iii)) uses the corresponding uncoupled atmosphere (ocean) tangent linear and adjoint model. There is no exchange of information between the two systems at any stage; the SST used at the atmosphere bottom boundary and the momentum, heat and freshwater fluxes at the ocean surface boundary are prescribed. Although this approach has its advantages, such as ease of implementation and modularity, it does not allow for cross-covariances between the atmosphere and ocean fields and atmospheric (ocean) observations cannot influence the ocean (atmosphere) analysis. The lack of feedback means that the atmosphere and ocean analysis states are unlikely to be in balance and this can have a negative impact if they are used to initialise a coupled model forecast (Balmaseda and Anderson, 2009).

2.1.3 Weakly coupled incremental 4D-Var

The weakly coupled assimilation system uses a coupled full state vector but uncoupled atmosphere

where is the prognostic variable, $_a$

3.4 Non-linear model validation

As part of the assimilation system development, the simplified non-linear model was validated against the ECMWF full physics version of the SCM code. As expected, we see small differences in the evolution of both the prognostic variables and surface fluxes but in general we find that using the simplified physics provides a good approximation to the full physics in the coupled model. Where there are differences the simplified model still produces an evolution that is physically reasonable, with a diurnal cycle in the ocean SST and mixed layer depth and appropriate atmosphere-ocean fluxes. We are therefore confident that the model is sufficient for assessing the different assimilation strategies.

Initial ocean elds are produced by interpolating Mercator Ocean reanalysis data[2] onto the KPP model grid. The surface short and long wave radiation forcing elds are computed by running the full physics version of the coupled single column model and taking 6 hourly snapshots of the diagnostic clear-sky radiation ux elds that are computed as part of the radiation scheme (ECMWF IFS documentation, 2001{2013b). The geostrophic components of the ocean currents (section 3.2.1) are estimated by computing a 10 day rolling average of the Mercator ocean currents. The surface heat, moisture and momentum uxes required for uncoupled ocean model integrations are taken from the ERA Interim Re-analysis.

For the experiments presented here, the true initial state is a 24 hour coupled model forecast valid at 00:00 UTC on 3rd June 2013 for the point (18875 E, 25 N) which is located in the north west Paci c ocean. This forecast was initialised using ERA interim and Mercator Ocean reanalysis data; we run a forecast rather than initialise from these data directly in order to generate an initial state that is consistent with the coupled model dynamics.

4.2 Background

The initial background state is generated by running a second 24 hour coupled model forecast from perturbed initial data; this data, denoted $\hat{x}$ $_{24}$x to modify the prior background error variance estimates and induce non-zero correlations between model variables.

A notable aspect in the ocean analysis errors is at approximately 20m, which coincides with the mixed layer depth. The mixed layer depth is characterised by a sharp gradient in the temperature and salinity profiles. In the background estimate the position of this feature is incorrect. When the assimilation of observations attempts to correct this positional error, instead of shifting the profiles, it erroneously changes the structure of the temperature and salinity profiles so that the error in the analysis is actually increased compared to the background. This is an issue for all three coupling strategies and is a well documented problem in the atmosphere when assimilating observations of the analogous boundary layer capping inversion (Fowler et al., 2012).

It is not possible to draw conclusions on the performance of each approach from the analysis errors alone. In particular, these results do not give any indication of whether the initial atmosphere and ocean analysis states are in balance. Since one of the key drivers behind the development of coupled data assimilation systems is generation of a consistent system state for the initialisation of coupled model forecasts, we use the t_0 analysis fields from each assimilation to initialise a series of coupled model forecasts; the results are discussed in sections 5.1 to 5.3.

5.1 Initialisation shock

A major problem with using analysis states from uncoupled assimilation systems to initialise a coupled model forecast is that the atmosphere and ocean fields may not be balanced and this can lead to initialisation shock. If the initial conditions are not on the coupled model attractor (in these twin experiments also the true attractor) the forecast will experience an adjustment process. In some cases the adjustment towards the model attractor solution occurs asymptotically but in others it manifests itself as a rapid change in the model fields in the early stages of the forecast (Balmaseda, 2012). The skill of a coupled model forecast depends strongly on the way it is initialised, thus the reduction or elimination of initialisation shock is particularly important in seasonal forecasting (Balmaseda and Anderson, 2009).

Figure 4 compares the SST and surface fluxes from each coupled model forecast against the truth trajectory and also a forecast initialised from the initial background state (i.e. no assimilation). In all cases, the forecast eventually tracks the true trajectory fairly well but there is variation in behaviour during the first part of the forecast window. There is evidence of initialisation shock in the SST field. The initial SST from the uncoupled ocean analysis is furthest from the true initial SST ($0.5\,$K warmer) and when the coupled model is initialised from the combined uncoupled atmosphere and ocean analysis states the forecast SST increases sharply, even further away from the true SST, over the first 5 model time-steps before gradually converging back towards the true trajectory. We also see jumps in the SST forecasts initialised from the strongly and weakly coupled analyses but these are much smaller suggesting that the coupled analyses are more balanced. In this example, the error in the weakly coupled SST analysis at the initial time is actually smaller than the strongly coupled SST analysis and the SST forecast from the weakly coupled analysis initially tracks the truth more closely. However, later in the forecast window, at the peak of the diurnal cycle ($25\,$hours), the SST forecasts from both the weakly and uncoupled analyses unexpectedly diverge from the truth, whereas the strongly coupled analysis continues to track it closely. This could be interpreted as a further indication of greater balance in the strongly coupled analysis; although the initial error in the SST forecast from the strongly coupled analysis is greater than the weakly coupled it appears to be in better balance with rest of the model. The error in the initial temperature at the bottom atmosphere level is very similar for all three forecasts but if we examine the atmosphere-ocean temperature difference (figure 5) we see that the strongly coupled system wind stress components (figure 4). The forecasts initialised from the weakly coupled and uncoupled analyses capture the general phasing of these fields but their magnitudes are overestimated to a greater extent than in the strongly coupled case over the first 24-48 hours of the forecast.

The latent heat flux forecasts are the slowest to stabilise; this is likely to be due to the fact that we are not assimilating observations of specific humidity. However, as the forecasts adjust towards the model attractor, there is a clear pattern of increasing accuracy as we progress from uncoupled to weakly to strongly coupled initialisation.

Overall our experiments have shown that, when compared to uncoupled initialisation, initialisa-

With single u and v wind observations only the u and v wind fields are updated at t_0 for both the strongly and weakly coupled systems. These initial wind increments do, however, produce increments to all of the atmosphere and ocean background fields over the remainder of the assimilation window. In this case, the strongly and weakly coupled analyses are identical; this is due to the model formulation and the fact that we are ignoring perturbations to the diffusion coefficients in the tangent and adjoint models as described in section 3.5. The u and v winds only depend on each other and so are essentially decoupled from the rest of the model in both the coupled model and atmosphere only model.

With u and v ocean surface current observations, the strongly coupled system produces initial increments in all fields, although these are very small for atmospheric temperature and specific humidity. The weakly coupled system only produces initial increments in the ocean fields and these are larger than in the strongly coupled case (figure 10). Again, the update of the initial state gives rise to increments in all fields across the assimilation window for both systems. Although the t_0 ocean analysis increments are larger in the weakly coupled system the increments across the assimilation window are generally smaller, particularly for the atmospheric fields, where there is no change to the initial states (results not shown). While there is no difference in the strongly and weakly coupled SST and surface fluxes when we assimilate single wind observations and only very small differences in the single SST observation experiment, for this case the strongly coupled system produces a much better analysis of the true surface wind stress and wind speed than the weakly coupled system (figure 11). The strongly coupled system is able to generate cross-covariances between the atmosphere and ocean fields and thus improve the wind analysis using the ocean current observations. Improved near-surface wind conditions can have a positive impact on air-sea exchange and thus both the atmosphere and ocean analyses. This result clearly demonstrates the potential for greater use of near surface data with strongly coupled assimilation.

These experiments have provided a valuable illustration of the ability of a strongly coupled assimilation system to induce cross-covariance information between the atmosphere and ocean variables, such that a single observation of a variable in one fluid at the end of the assimilation window can produce increments to variables in the other fluid at initial time t_0. Although the structure of the weakly coupled assimilation system does not allow atmosphere-ocean cross-covariances, there is benefit to be gained from this approach if more than one outer-loop is used, and particularly if improvement was clearly evident when using analyses from the strongly coupled system, it was not always so obvious with the weakly coupled system. The ability of the weakly coupled assimilation system to reduce initialisation shock was found to be sensitive to the input parameters, such as observation frequency and background error variances (not shown). In the best cases the behaviour of the SST and surface fluxes in the initial stages of the forecast (used to identify shock) followed those from the strongly coupled assimilation. In other cases the weakly coupled assimilation did not show the same improvement as strongly coupled assimilation. However, the weakly coupled system was usually comparable to uncoupled assimilations in which the atmosphere and ocean models were forced using the `true' SST and surface fluxes. This illustrates that even moving to a weakly coupled assimilation system is likely to have a benefit, as the update of the SST and surface fluxes through the outer-loop step can provide useful information not available to the uncoupled assimilation systems.

Single observation experiments were used to demonstrate how coupled assimilation systems offer the potential for improved use of near-surface observations via the generation of cross covariance information. Although the possible cross-covariances that can be generated are partly limited by the simplified dynamics of our model, the effect of coupled assimilation can clearly be seen. The strongly coupled assimilation system is able to implicitly induce cross-covariance information between the atmosphere and ocean at the initial time, such that a single ocean observation can generate analysis increments in the initial atmospheric fields and vice-versa. While the design of the weakly coupled incremental 4D-Var assimilation algorithm does not allow this, the use of the coupled model in the outer-loop update step means that if more than one outer-loop is run, an observation in one system can affect the other system by changing the linearisation state. Thus information from near-surface

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Table 1: observation error standard deviations by eld

atmosphere temperature (K)	u wind (ms ^{1})	v wind (ms ^{1})	ocean temperature (K)	salinity (psu)	u current (ms ^{1})	v current (ms ^{1})
1.0	1.5	1.5	0.01	0.003	0.01	0.01

Table 2: atmosphere observation locations

model level	standard pressure level (hPa)	model full level pressure value (hPa)[3]
14	10	9.893
17	20	18.815
19	30	28.882
22	50	54.624
23	70	66.623
25	100	95.980
28	150	154.038
30	200	202.230
32	250	257.685
33	300	288.093
36	400	389.233
39	500	501.637
44	700	694.696
49	850	861.497
52	925	935.065
56	1000	995.055
60	n/a	1017.293

[3] values based on a surface pressure value of 1018.5 hPa; model full level pressure values vary with surface pressure. These levels have been chosen to approximately correspond to the standard pressure levels (hPa).

Table 3: ocean observation locations

model level	depth (m)
1	1.000
3	3.069
5	5.277
8	8.848
10	11.406
13	15.538
16	20.173
18	23.762
20	28.100
22	33.760
23	37.366
24	41.703
25	46.985
26	53.475
27	61.498
28	71.452
29	83.818
30	99.175
31	118.214
32	141.758
33	170.778
34	206.414
35	250.000

Figure 2: Initial background (solid black line) and observation (dashed blue line) error standard deviations.

Figure 3: 12 hour assimilation window with 3 hourly atmosphere & 6 hourly ocean observations: Analysis errors at initial time solid black line: (truth-background); dashed red line: strongly coupled (truth-analysis); solid blue line: weakly coupled (truth-analysis); dot-dash green line: uncoupled (truth-analysis).

Figure 4: 12 hour assimilation window with 3 hourly atmosphere & 6 hourly ocean observations: coupled model SST & surface fluxes for coupled model forecast initialised from t_0 analyses. Solid black line: truth; solid grey line: forecast initialised from initial background state; dashed red line: initial condition is strongly coupled analysis; solid blue line:

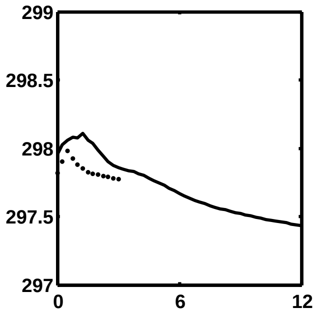

Figure 6: 12 hour assimilation window with 3 hourly atmosphere & 6 hourly ocean observations: coupled model SST & surface uxes for coupled model forecast initialised from t_0 analyses. Solid black line: truth; dashed red line: initial condition is strongly coupled analysis; solid blue line: initial condition is weakly coupled analysis; dot-dash green line: initial condition is uncoupled analysis; black dots: initial condition is analysis from uncoupled assimilations with `true' forcing.

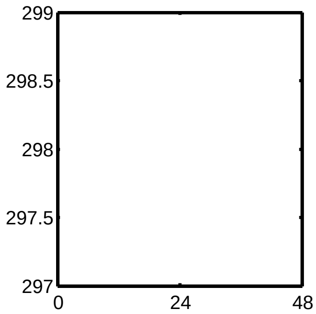

Figure 7: 12 hour assimilation window with 6 hourly atmosphere & ocean observations: coupled model SST & surface uxes for coupled model forecast initialised from t_0 analyses. Solid black line: truth; dashed red line: initial condition is strongly coupled analysis; solid blue line: initial condition is weakly coupled analysis; dot-dash green line: initial condition is uncoupled analysis.

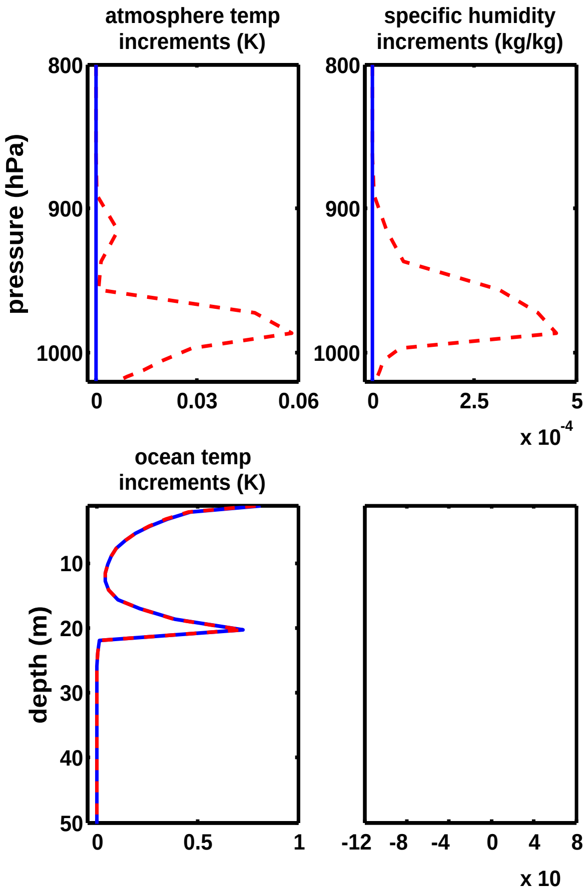

Figure 8: Analysis increments at t = 0: single SST observation at end of 12 hour assimilation window. Dashed red line: strongly coupled assimilation; solid blue line: weakly coupled assimilation.

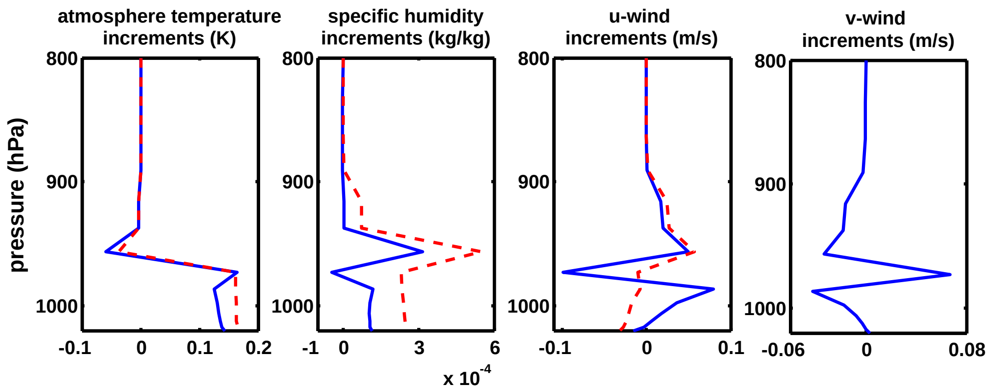

Figure 9: Analysis increments at t = 6 hr: single SST observation at end of 12 hour assimilation window. Dashed red line: strongly coupled assimilation; solid blue line: weakly coupled assimilation.

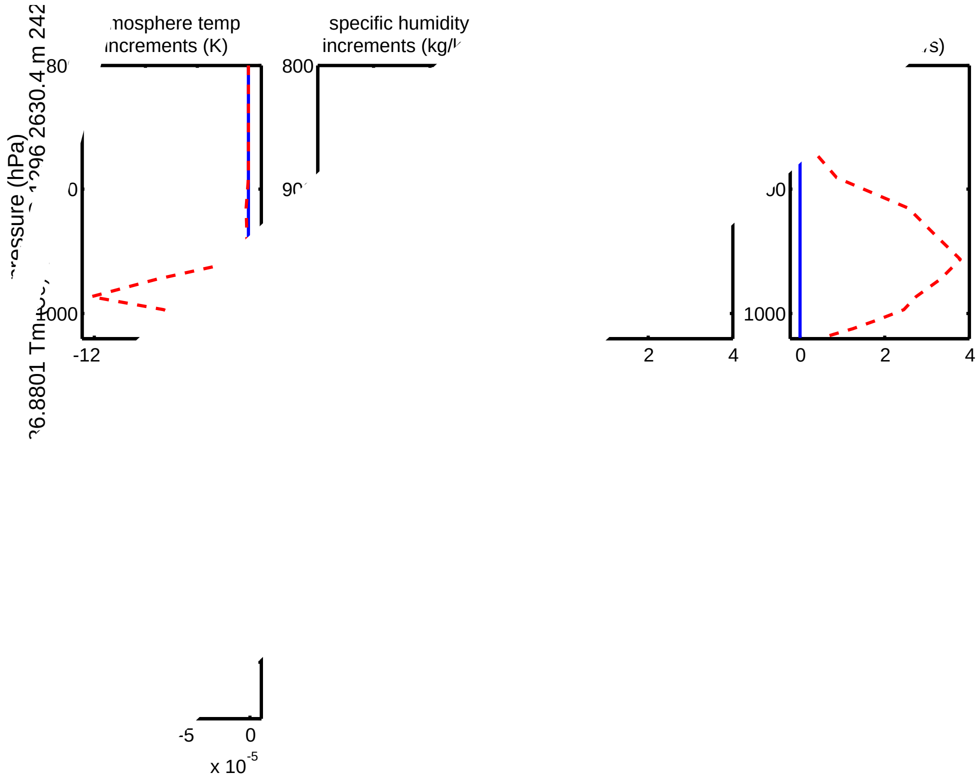

Figure 10: Analysis increments at t = 0: single ocean surface current observation at end of 12 hour assimilation window. Dashed red line: strongly coupled assimilation; solid blue line: weakly coupled assimilation.

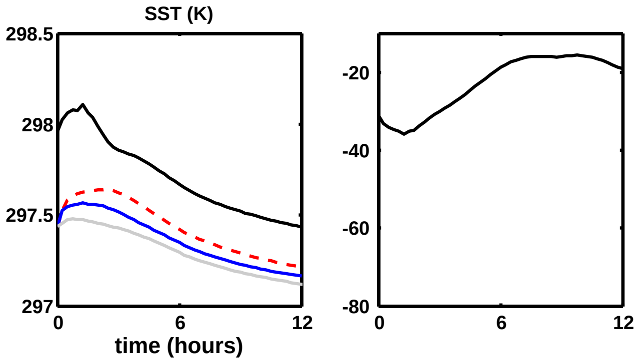

Figure 11: SST and surface uxes: single ocean surface current observation at end of 12 hour assimilation window. Solid black line: truth; solid grey line: background; dashed red line: strongly coupled assimilation; solid blue line: weakly coupled assimilation.