

Mediating scale separation in Strongly Coupled Data Assimilation

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Abstract

Data Assimilation (DA) in a simple coupled system set-up is explored using linear and non-linear coupled toy models capturing the macroscopic properties of the ocean-atmosphere interactions. We especially concentrate on the effects of temporal scale separation between the oceanic and atmospheric sub-components, and its effects on the optimal implementation and possible modifications at the zeroth order to the typical DA procedures employed in weather forecasting and climate prediction.

1 Introduction

Data Assimilation (*abbrev.* DA), broadly speaking, is a conceptual and mathematical framework that aims to combine the information from observational datasets with the predictions from proposed model forms in order to yield a ‘true’ estimate of the state; the ‘true’ state in this case refers to the derived state that is a more accurate representation of the system than what is predicted by the model, or implied by the observations, independently. In some sense, DA could be interpreted as a propagation of an initial forecast state predicted by a given model towards higher likelihood by *assimilating* the observations. In context of complex earth systems, DA has been long utilised in geosciences, especially in meteorology and weather prediction [2], climate change [3], and more recently in attempting long-term climate prediction [7]. In this paper, we will concentrate on the application of DA to meteorology – often interpreted as accurate forecasts on short time-scales ($\lesssim 2$ weeks), and climate prediction – on time-scales longer than typical range covered by meteorology or weather prediction ($\gtrsim 2$ weeks). In such earth systems, the proposed models are typically dynamic, high-dimensional and qualitatively error-prone due to the inherent complexity in modelling the system. In particular, the dynamic nature of the models result in a discrete and sequential implementation of DA in time [2]; this essentially differentiates DA from a matched-filtering procedure where the model forms are deterministic and incorporate explicit time-dependence.

Theoretically speaking, the complexity – and accuracy – of DA for a given system is shared by the intrinsic complexity in the model form (e.g. model degrees of freedom, participating sub-systems, etc) as well as the nature of observations (e.g. the spatial and temporal scarcity of data points, accuracy of the observational datasets, etc). In practice, however, limitations on DA due to the nature of observational datasets are largely systematic and extrinsic, while the impact of the model form has a more fundamental and profound impact. In this respect, the case of coupled systems is extremely

relevant and interesting since it presents with a realistic challenge where the model form of the system entails two or more sub-components with differing time-scales, e.g. ocean-atmosphere coupled earth system. This has a fundamental impact on the accuracy of DA on each observed sub-component on any intended time-scale and to varying magnitudes [7, 8]. In this paper, we will study the effects of multi-component coupling in the model form on the DA procedure using two toy models capturing the macroscopic properties of ocean-atmosphere interactions – one linear, and one non-linear and chaotic. The intention, in the end, is to develop a zero-order treatment of sequential coupled data assimilation and possible modifications to it in the linear as well as non-linear and chaotic regime.

2 Linear coupled model

The linear toy model M_{lin} for the first case study is adopted from Barsugli and Battisti [1], which is a simple one-dimensional, thermally coupled, purely temporal and stochastically forced atmosphere-ocean system of the form

$$m \frac{dT_O}{dt} = C_{OO} T_O + C_{OA} T_A, \quad (1)$$

$$\frac{dT_A}{dt} = C_{AO} T_O + C_{AA} T_A + F(t). \quad (2)$$

In matrix form, the coupled system may be written as

$$\nabla \mathbf{T} = \mathbf{C} \mathbf{T} + \mathbf{F}, \text{ where,} \quad (3)$$

$$\nabla = \begin{bmatrix} m \frac{d}{dt} & \emptyset \\ \emptyset & \frac{d}{dt} \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} T_A \\ T_O \end{bmatrix},$$

$$\mathbf{C} = \begin{bmatrix} C_{OO} & C_{OA} \\ C_{AO} & C_{AA} \end{bmatrix}, \text{ and } \mathbf{F} = \begin{bmatrix} F(t) \\ \emptyset \end{bmatrix}. \quad (4)$$

where $\mathbf{T} = [T_O, T_A]$ is the state vector of the temperature anomalies in the ocean and atmosphere respectively, matrix \mathbf{C} encodes the exchange of information between the two sub-components, ‘ m ’ encodes the temporal scale separation between the two sub-components, ∇ is the

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translation operator and $F(t)$ is the stochastic forcing term. We choose the members of \mathbf{C} and the value of scale separation ‘ m ’ such that the system is stable and in dynamic thermal equilibrium, e.g. $C_{OO} = -0.1$, $C_{OA} = 0.1$, $C_{AO} = 0.01$ and $C_{AA} = -0.1$, and ocean is relatively slow evolving ($m > 1$). The stability of the system is ensured by negative eigenvalues of $\mathbf{C} \leftrightarrow |\mathbf{C}| > 0 \leftrightarrow \mathbf{C}$ is positive definite, which also ensures that the Lyapunov exponents are negative. The presence of the forcing term ensures that the model is dynamically spun up to mimic realistic scenarios and its cross-section σ_F is chosen accordingly. In figure 1, we show a sample time series for a single member simulation.

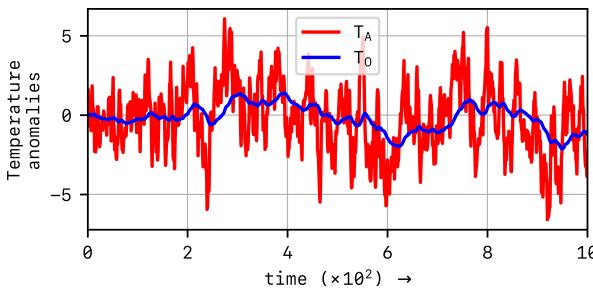


Figure 1: 1-member simulation for $m = 10$, $\sigma_F = 0.1$, and $T_O^{t=0} = T_A^{t=0} = 0.0$.

One may easily calculate the frequency spectrum of the solutions ($t \rightarrow f$) in the Fourier space analytically in this case (5), to quantify the relative slowness of the ocean with respect to the atmosphere; this is shown in figure 2 – the gap between the Fourier transforms \hat{T}_O and \hat{T}_A quantifies the slowness of the ocean relative to the atmosphere.

$$\begin{aligned}\hat{T}_O(f) &= \sigma_F^2 \frac{C_{OA}}{(2\pi i f - C_{AA})(2\pi i m f - C_{OO}) - C_{OA}C_{AO}} \\ \hat{T}_A(f) &= \sigma_F^2 \frac{2\pi i m f - C_{OO}}{(2\pi i f - C_{AA})(2\pi i m f - C_{OO}) - C_{OA}C_{AO}}\end{aligned}\quad (5)$$

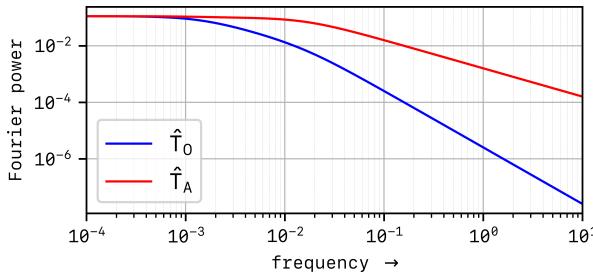


Figure 2: Fourier transforms \hat{T}_O and \hat{T}_A for $m = 10$, $\sigma_F = 0.1$.

Lastly, this temporal scale separation (i.e. slowness of the ocean) leads to a net lagging effect on the ocean which is quantifiable by calculating the auto- and cross-

correlation functions (6).

$$\langle T_X, T_Y \rangle \equiv \langle T_X(t), T_Y(t + \tau) \rangle = \int_{-\infty}^{+\infty} T_X(t) T_Y(t + \tau) dt. \quad (6)$$

where τ is the *lag time*. In figure 3, we show the auto- and cross-correlation functions plotted for our linear model where the slowness of ocean is again reflected in shallower decline of the oceanic auto-correlation function $\langle T_O, T_O \rangle$ relative to the atmospheric auto-correlation function $\langle T_A, T_A \rangle$. Notably, the cross-correlation function $\langle T_O, T_A \rangle$ peaks at negative value of τ (denoted by τ_p) depicting that the ocean *lags* the atmosphere, or that the atmosphere *leads* the ocean. We intend to use this lag to our advantage in the data assimilation procedure. The statistics of $|\tau_p|$ as a function of scale separation ‘ m ’ are shown in figure 4; we find that the modes of the distributions (i.e. values of $|\tau_p|$) increase with increasing scale separation (i.e. ‘ m ’) as expected. Moreover, while $|\tau_p|$ primarily depends on ‘ m ’ and $|\mathbf{C}|$, the higher moments (skewness, kurtosis, etc) depend on $\mathbf{C} - \text{diag}(\mathbf{C})$.

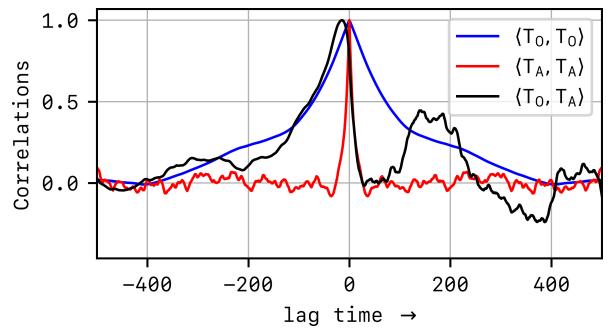


Figure 3: Cross- and auto-correlation functions $\langle T_X, T_Y \rangle$ for a 1-member simulation for $m = 10$, $\sigma_F = 0.1$, and $T_O^{t=0} = T_A^{t=0} = 0.0$. Note that the auto-correlation functions naturally peak at $\tau = 0$ while the cross-correlation peaks at $\tau < 0$ depicting the *lagging effect* on the ocean.

2.1 DA on the linear model

In order to study and optimise data assimilation using this coupled linear model M_{lin} , we utilise the existing framework of sequential *Ensemble Kalman Filter* (abbrev. EnKF); it is a well known fact that in the linear case, EnKF is the most optimal choice for data assimilation considering the analytical constraints as it equates to a unique and global minimisation of the standard variational approach [2]. If the model error covariance matrix is denoted by \mathbf{P} , the observational error covariance matrix by \mathbf{R} , then the Kalman Gain \mathbf{K} at any time t is written as

$$\mathbf{K}_t = \mathbf{P}_t [\mathbf{P}_t + \mathbf{R}_t]^{-1}. \quad (7)$$

The resulting analysed and forecast state at any time t are further written as

$$\mathbf{T}_t^{\text{ana}} = \mathbf{T}_t^{\text{for}} + \mathbf{K}_t [\mathbf{T}_t^{\text{obs}} - \mathbf{T}_t^{\text{for}}], \quad (8)$$

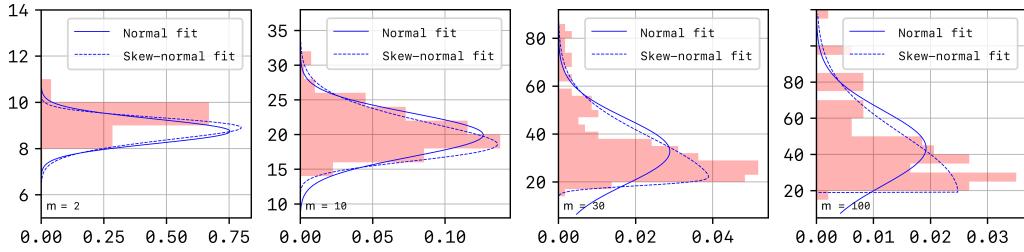


Figure 4: Normalised probability densities (horizontal axes) of peak lag times $|\tau_p|$ (vertical axes) as a function of scale separation ‘ m ’. $\sigma_F = 0.1$, and $T_O^{t=0} = T_A^{t=0} = 1.0$. The solid lines denote normal distribution fits while the dashed lines denote skew-normal fits. Note the shift in the mode, the skewness and the spread of the distributions as a function of increasing values of $m \in \{2, 10, 30, 100\}$.

where $\mathbf{T}_t^{\text{obs}}$ and $\mathbf{T}_t^{\text{for}}$ are the observation and forecast vectors. The analysed model error covariance matrix evolves as $\mathbf{P}_t^{\text{ana}} = \mathbf{P}_t^{\text{for}} [\mathbf{I} - \mathbf{K}_t]$ although this calculation is not required explicitly by the ensemble version of the Kalman filter. The analysed state $\mathbf{T}_t^{\text{ana}}$ is finally translated in time from t to $t+1$ by the translation operation, $\mathbf{T}_{t+1}^{\text{for}} = \mathcal{M}_{\text{lin}} \cdot \mathbf{T}_t^{\text{ana}}$, by numerically integrating the coupled stochastic differential equations¹ (1)–(2). In our experiments, we reasonably assume the observation errors in the ocean and the atmosphere to be mutually uncorrelated and constant in time², i.e.

$$\mathbf{R}_t = \begin{bmatrix} \sigma_{A, \text{obs}} & \emptyset \\ \emptyset & \sigma_{O, \text{obs}} \end{bmatrix}_{\forall t}, \quad (9)$$

$$\mathbf{K}_t = \frac{1}{D_t} \begin{bmatrix} \langle \vec{T}_A^{\text{for}} | \vec{T}_A^{\text{for}} \rangle [\langle \vec{T}_O^{\text{for}} | \vec{T}_O^{\text{for}} \rangle + \sigma_{O, \text{obs}}^2] - \langle \vec{T}_O^{\text{for}} | \vec{T}_A^{\text{for}} \rangle^2 \\ \sigma_{A, \text{obs}}^2 \langle \vec{T}_A^{\text{for}} | \vec{T}_O^{\text{for}} \rangle \end{bmatrix}$$

while the model error covariance matrix \mathbf{P}_t is explicitly written as

$$\mathbf{P}_t = \begin{bmatrix} \langle \vec{T}_A^{\text{for}} | \vec{T}_A^{\text{for}} \rangle & \langle \vec{T}_A^{\text{for}} | \vec{T}_O^{\text{for}} \rangle \\ \langle \vec{T}_O^{\text{for}} | \vec{T}_A^{\text{for}} \rangle & \langle \vec{T}_O^{\text{for}} | \vec{T}_O^{\text{for}} \rangle \end{bmatrix}_t. \quad (10)$$

The observation vectors for the ocean and the atmosphere in our experiments are generated by perturbing a 1-member simulation of the model \mathcal{M}_{lin} with $\sigma_{O, \text{obs}}$ and $\sigma_{A, \text{obs}}$ respectively. Lastly, the Kalman Gain matrix \mathbf{K}_t is explicitly written as

$$\begin{bmatrix} \sigma_{O, \text{obs}}^2 \langle \vec{T}_O^{\text{for}} | \vec{T}_A^{\text{for}} \rangle \\ \langle \vec{T}_O^{\text{for}} | \vec{T}_O^{\text{for}} \rangle [\langle \vec{T}_A^{\text{for}} | \vec{T}_A^{\text{for}} \rangle + \sigma_{A, \text{obs}}^2] - \langle \vec{T}_A^{\text{for}} | \vec{T}_O^{\text{for}} \rangle^2 \end{bmatrix}_t, \quad (11)$$

Parameter	Value	Parameter	Value
m	$\in [1, 10]$	τ	$\in [0, 41]$
$T_O^{t=0}$	0.0	$T_A^{t=0}$	0.0
$\sigma_{O, \text{for}}^{t=0}$	1.0	$\sigma_{A, \text{for}}^{t=0}$	2.0
$\sigma_{O, \text{obs}}$	1.0	$\sigma_{A, \text{obs}}$	2.0
σ_F	1.0	N_e	25

Table 1: Values of the parameters

where $D_t = [\langle \vec{T}_A^{\text{for}} | \vec{T}_A^{\text{for}} \rangle + \sigma_{A, \text{obs}}^2] [\langle \vec{T}_O^{\text{for}} | \vec{T}_O^{\text{for}} \rangle + \sigma_{O, \text{obs}}^2] - \langle \vec{T}_O^{\text{for}} | \vec{T}_A^{\text{for}} \rangle^2$, and $\vec{\cdot}$ represents the ensemble vector of length N_e , the time-varying spread of the ensembles is denoted by $\sigma_{A/O, \text{for/ana}}$, and the $\langle \cdot | \cdot \rangle$ operation represents inner product. Naturally, $\langle \vec{T}_O^{\text{for}} | \vec{T}_A^{\text{for}} \rangle = \langle \vec{T}_A^{\text{for}} | \vec{T}_O^{\text{for}} \rangle$ and that $\langle \vec{T}_X^{\text{for}} | \vec{T}_Y^{\text{for}} \rangle$ is generally equivalent to the dis-

crete formulation of the zero-lag correlation function $\langle T_X | T_Y \rangle_{\tau=0}$ in (6). This completes the required ingredients for EnKF. In table 1, we list the values of the parameters defined above.

We quantify the performance of DA by calculating the RMSE vector defined by

$$\sigma_{\text{RMSE}} = \sqrt{\sum_{\forall t} |\mathbf{T}_t^{\text{obs}} - \mathbf{T}_t^{\text{ana}}|^2}. \quad (12)$$

In standard large-scale data assimilation applications, a *strongly* coupled approach (*abbrev.* SCDA) as outlined above is not yet adopted although its application has been encouraged in recent times [6]. The current adoption of *weakly* coupled implementation (*abbrev.* WCDA) simply involves setting the off-diagonal terms in \mathbf{P}_t to zero, thereby explicitly ignoring the model error covariances in the analysis step and only allowing the coupled system to share information during the forecast step; this approach is prone to instabilities. In order to show the difference between the two, we run WCDA simulations

¹The expression (3) is of the *Ito* form and its numerical integration is performed using `sdeint.itoint` algorithm available in Python’s SciPy library. More specifically, `sdeint.itoint` uses the Euler-Maruyama algorithm to integrate the Ito equation.

²We use the explicit form of \mathbf{R} in our simulations instead of the ensemble form for simplicity.

in parallel with SCDA in all our experiments and calculate $\delta\sigma_{\text{RMSE}} = \sigma_{\text{RMSE}}^{\text{SCDA}} - \sigma_{\text{RMSE}}^{\text{WCDA}}$. In figure 5, we show a snapshot of a random ensemble member's simulation while figure 6 shows the corresponding RMSE statistics derived from a 25-member EnKF simulation by fixing $m = 10$.

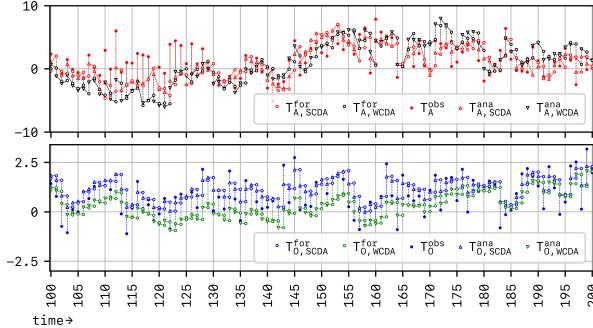


Figure 5: One random member EnKF simulation for $m = 10$ showing the WCDA and the SCDA implementations. Top panel (red) shows the atmospheric component while the bottom panel depicts the ocean (blue).

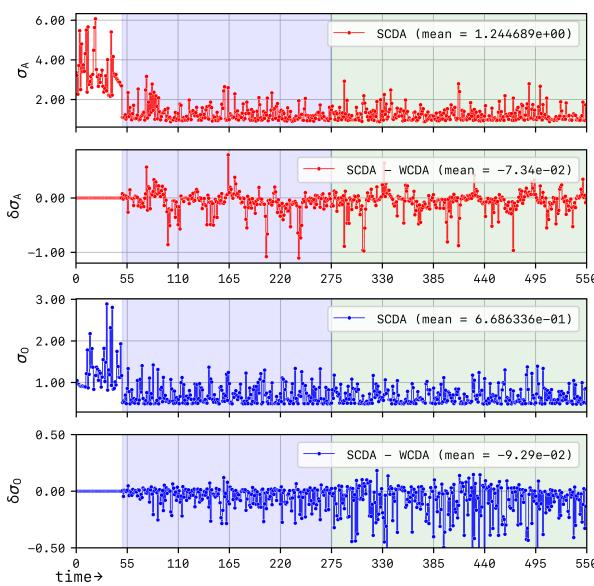


Figure 6: RMSE statistics derived from a 25-member EnKF simulation of the SCDA ($\sigma_{A/O}$), and the difference between the WCDA and the SCDA implementation ($\delta\sigma_{A/O}$); $m = 10$. The model is spun up to stability during time $t \in [0, 50]$ whereas the RMSE means are calculated for time $t \in (275, 550]$. In this particular experiment, SCDA seems to perform marginally better than WCDA although this discrepancy is much smaller than the climatological background error due to the stochastic forcing term and should not be over-emphasised.

Inflation

We note that the spread of the ensemble in our simulation contracts over time since the model error covariance matrix evolves as $\mathbf{P}_t^{\text{ana}} = \mathbf{P}_t^{\text{for}} [\mathbf{I} - \mathbf{K}_t]$ besides the usual variation due to the model flow [2]. This leads to convergence issues and degradation in the performance of

DA over time; we counter this effect by, *a*) adaptively inflating the individual ensembles in the ocean and the atmosphere by a time-dependent factor $\alpha_t^{O/A}$ such that the ensemble spread is preserved between the forecast and the analysis step, and *b*) secondary multiplicative inflation of the ensemble for SCDA simulation by a constant factor γ , applied to both the oceanic as well as the atmospheric ensemble, on top of the adaptive inflation.

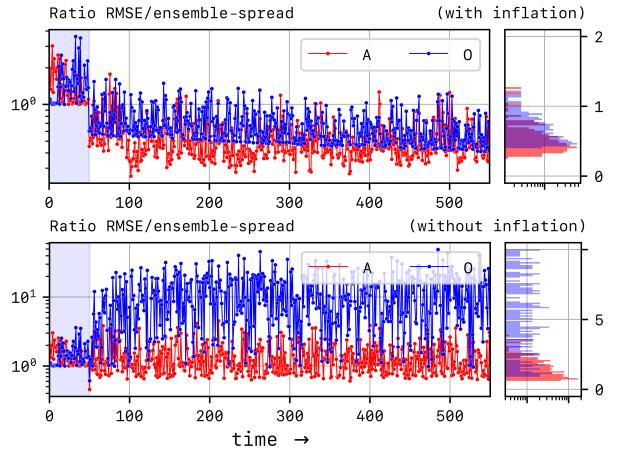


Figure 7: The convergence of SCDA is probed by calculating the ratio between the RMSE and the spread of the ensemble for each sub-component over time t for $m = 10$. The criteria of convergence requires that this ratio tends to $\lesssim 1$ in the limit $t \rightarrow \infty$. We find that inflation is necessary to achieve convergence for both SCDA and WCDA (not shown).

The mean values $\bar{\alpha}_m^{O/A}$ of the multiplicative inflationary factor α_t over time for a given ' m ' is shown in figure 8 (bottom panel). It is noteworthy that the adaptive multiplicative inflation counters the contraction of ensemble due to the DA while the constant multiplicative inflation counters the deflation of ensemble due to the dissipative nature of the model. Thus, it follows that γ must depend on the choice of ' m ' in the model. In particular, γ must decrease monotonically with increasing value of ' m '; we ran a tuning simulation to optimise the choice of γ_m and its results are shown in figure 8 (top panel).

2.2 Leading averaged cross-covariance

In order to maximise the effects of cross-covariance in coupled data assimilation, Lu *et al* [4, 5] suggested that it is advantageous to use leading forecasts and observations in the fast sub-component, i.e. the atmosphere, while updating the slower sub-component, i.e. the ocean, instead of assimilating the instantaneously available atmospheric observation at any time t . This suggestion simply follows from figure 3 where we found that the cross-correlation function is maximum when atmosphere leads the ocean, i.e. when $\tau < 0$. This essentially means that the information shared between the oceanic and the atmospheric sub-components in the cross-update may be optimised further by choosing

$\tau < 0$, thus maximising the signal-to-noise ratio (SNR) in the cross-update. In order to further minimise the effects of noise arising due to stochastic forcing, Lu *et al* [4] used an average over some τ_{win} number of leading observations in the atmosphere to update the ocean; they termed this implementation as LACC [4, 5]. Note that no modification was necessary in reverse, i.e. ocean \rightarrow atmosphere, since the faster sub-component doesn't benefit from any such modification directly.

In this paper, we will attempt to quantify the effects of choices of τ_{win} on $\delta\sigma_{\text{RMSE}}$. It must be noted that the optimal choice of τ_{win} must depend on ‘m’ since $|\tau_p|$ depends on ‘m’. Consequently, the results of the LACC implementation compared with the WCDA and the SCDA are shown in figure 9 as a function of ‘m’ and τ_{win} . In principle, we expect that for larger scale separations, correspondingly longer leading averaged windows should maximise the cross-component SNR, thus leading to a larger disparity between the LACC and the SCDA/WCDA implementations. However, we note that longer window lengths also decrease the frequency of the coupled cross-updates since this update is made only when preceding τ_{win} observations in the atmosphere become available, which contribute toward diminishing returns of LACC as seen in figure 9. Overall, we find that the LACC method performs better than the standard WCDA and SCDA implementations in the ocean when the noise is not too overwhelming. In particular, the impact of the frequency of stochastic forcing on the slower ocean sub-

component is detrimental to the extent that LACC and SCDA perform worse than WCDA in some cases whereas the atmosphere doesn't suffer from such an effect (i.e. WCDA is globally worse).

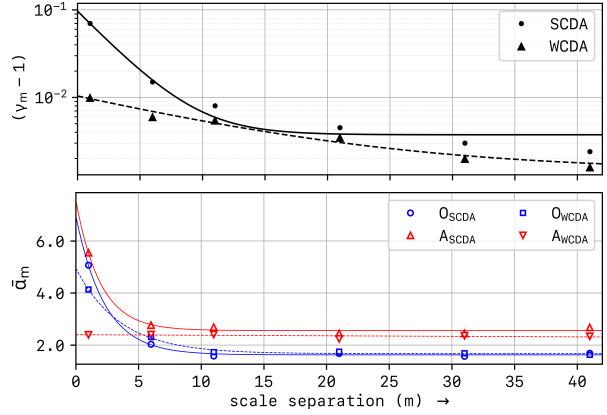


Figure 8: Top panel: Calculated values of γ_m are shown on the vertical axes for different choices of scale separation on the horizontal axes. We fit the data points with decaying exponential functional forms, where solid (—) and dashed (--) lines represent the SCDA and the WCDA respectively, in order to derive a generalised analytical expression; using this formulae, we calculate the optimal choices of γ_m for any given ‘m’. Bottom panel: Mean values over time of the adaptive multiplicative inflation, i.e. $\bar{\alpha}_m^{O/A}$, are shown for different choices of scale separation for individual sub-components in the SCDA and the WCDA implementation.

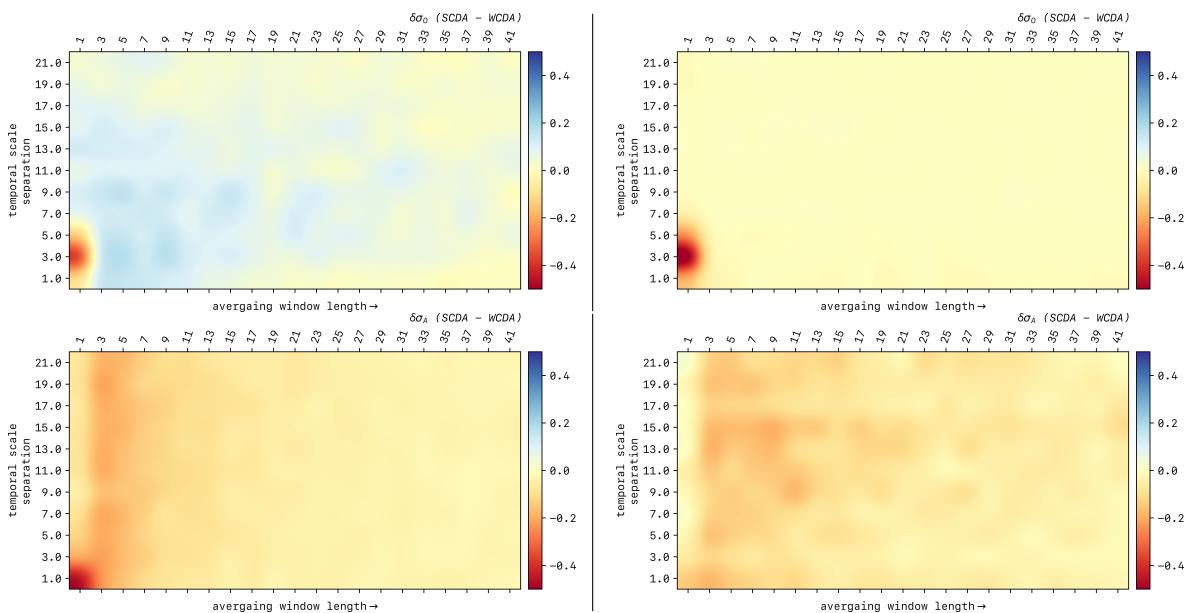


Figure 9: RMSE statistics derived from a 25-member EnKF simulation as a function of ‘m’ (vertical axes) and τ_{win} (horizontal axes) showing the difference between the WCDA and the LACC implementation (including fully adaptive inflation with γ_m and $\alpha_{t,m}$). The top panel shows the oceanic component while the bottom panel depicts the atmosphere. Note that the SCDA case depicted in figures 5–6 corresponds to $\tau_{\text{win}} = 1$ in this plot. In order to compare the effect of frequency of stochastic forcing, we include the simulation results for when the forcing is applied every 10 time steps (right column) instead of every iteration (left column); note the higher efficiency of the SCDA implementation in the case of former less frequent stochastic forcing.

3 Extension of LACC to non-linear case

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