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Data-driven Interpolation of Sea Level Anomalies using Analog Data Assimilation

Redouane Lguensat^{a,*}, Phi Huynh Viet^a, Miao Sun^b, Ge Chen^b, Tian Fenglin^b, Bertrand Chapron^c, Ronan Fablet^a

^aIMT Atlantique, Lab-STICC, Université Bretagne Loire ^bDepartment of Marine Technology, College of Information Science and Engineering, Ocean University of China, Qingdao, China ^cLaboratoire d'Océanographie Physique et Spatiale, Centre de Brest, IFREMER, Plouzané, France

Abstract

Despite the well-known limitations of Optimal Interpolation (OI), it remains the conventional method to interpolate Sea Level Anomalies (SLA) from altimeter-derived along-track data. In consideration of the recent developments of data-driven methods as a means to better exploit large-scale observation, simulation and reanalysis datasets for solving inverse problems, this study addresses the improvement of the reconstruction of higher-resolution SLA fields using analog strategies. The reconstruction is stated as an analog data assimilation issue, where the analog models rely on patch-based and EOF-based representations to circumvent the curse of dimensionality. We implement an Observation System Simulation Experiment in the South China sea. The reported results show the relevance of the proposed framework with a significant gain in terms of root mean square error for scales below 100km. We further discuss the usefulness of the proposed analog model as a means

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^{*}corresponding author, email: redouane.lguensat@imt-atlantique.fr

to exploit high-resolution model simulations for the processing and analysis of current and future satellite-derived altimetric data. *Keywords:* Analog Data Assimilation, Sea Level Anomaly, Sea Surface Height, Interpolation, Data-driven methods

1 1. Introduction

The past twenty years have witnessed a deluge of ocean satellite data, such as sea surface height, sea surface temperature, ocean color, ocean current, sea ice, etc. This has helped building big databases of valuable information and represents a major opportunity for the interplay of ideas between ocean remote sensing community and the data science community. Exploring machine learning methods in general and non-parametric methods in particular is now feasible and is increasingly drawing the attention of many researchers (Zhang et al., 2016; Lary et al., 2016).

More specifically, analog forecasting (Lorenz, 1969) which is among the 10 earliest statistical methods explored in geoscience benefits from recent ad-11 vances in data science. In short, analog forecasting is based on the assump-12 tion that the future state of a system can be predicted throughout the succes-13 sors of past (or simulated) similar situations (called analogs). The amount of 14 currently available remote sensing and simulation data offers analog methods 15 a great opportunity to catch up their early promises. Several recent works 16 involving applications of analog forecasting methods in geoscience fields con-17 tribute in the revival of these methods, recent applications comprise the pre-18 diction of soil moisture anomalies (McDermott and Wikle, 2015), the predic-19 tion of sea-ice anomalies (Comeau et al., 2017), rainfall nowcasting (Atencia 20

and Zawadzki, 2015), stochastic weather generators (Yiou, 2014), etc. One 21 may also cite methodological developments such as dynamically-adapted ker-22 nels (Zhao and Giannakis, 2014a) and novel parameter estimation schemes 23 (Horton et al., 2017). Importantly, analog strategies have recently been ex-24 tended to address data assimilation issues within the so-called *analog data* 25 assimilation (AnDA) (Lguensat et al., 2017), where the dynamical model 26 is stated as an analog forecasting model and combined to state-of-the-art 27 stochastic assimilation procedures such as Ensemble Kalman filters. The re-28 cent applications to high-dimensional fields in Fablet et al. (2017) provide 29 the methodological background for this study. 30

Producing time-continuous and gridded maps of Sea Surface Height (SSH) 31 is a major challenge in ocean remote sensing with important consequences 32 on several scientific fields from weather and climate forecasting to opera-33 tional needs for fisheries management and marine operations (e.q. Hardman-34 Mountford et al. (2003)). The reference gridded SSH product commonly used 35 in the literature is distributed by the Copernicus Marine and Environment 36 Monitoring Service (CMEMS) (formerly distributed by AVISO). This prod-37 uct relies on the interpolation of irregularly-spaced along-track data using an 38 Optimal Interpolation (OI) method (Le Traon et al., 1998; Bretherton et al., 39 1976). While OI is relevant for the retrieval of horizontal scales of SSH fields 40 greater than $\approx 100 km$, its Gaussian assumptions cause the small scales of the 41 SSH fields to be smoothed. This limitation makes it impossible to resolve 42 finer-scale processes (typically from a few tens of kilometers to $\approx 100 km$) 43 which may be revealed by along-track altimetric data. This has led to a 44 variety of research studies to improve the reconstruction of the altimetric fields. One may cite both methodological alternatives to OI, for instance
locally-adapted convolutional models (Fablet et al., 2016) and variational assimilation schemes using model-driven dynamical priors (Ubelmann et al.,
2014), as well as studies exploring the synergy between different sea surface
tracers, especially the synergy between SSH and SST (Sea Surface Temperature) fields and Surface Quasi-Geostrophic dynamics (Fablet et al., 2016;
Klein et al., 2009; Isern-Fontanet et al., 2006, 2014; Turiel et al., 2009b,a).

In this work, we build upon our recent advances in analog data assimi-53 lation and its application to high-dimensional fields (Lguensat et al., 2017; 54 Fablet et al., 2017). We develop an analog data assimilation model for the 55 reconstruction of SLA fields from along-track altimeter data. It relies on a 56 patch-based and EOF-constrained representation of the SLA fields. Using 57 OFES numerical simulations (Masumoto et al., 2004; Sasaki et al., 2008), 58 we design an Observation System Simulation Experiment (OSSE) for a case-59 study in the South China sea using real along-track sampling patterns of 60 spaceborne altimeters. Using the resulting groundtruthed dataset, we per-61 form a qualitative and quantitative evaluation of the proposed scheme, in-62 cluding comparisons to state-of-the-art schemes. 63

The remainder of the paper is organized as follows: Section 2 presents the different datasets used in this paper to design an OSSE, Section 3 gives insights on the classical methods used for mapping SLA from along track data, Section 4 introduces the proposed analog data assimilation model. Experimental results for the considered OSSE are shown in Section 5, and Section 6 further discuss the key aspects of this work.

70 2. Data: OFES (OGCM for the Earth Simulator)

An Observation System Simulation Experiment (OSSE) based on numerical simulations is considered to assess the relevance of the proposed analog assimilation framework. Our OSSE uses these numerical simulations as a groundtruthed dataset from which simulated along-track data are produced. We describe further the data preparation setup in the following sections.

76 2.1. Model simulation data

The Ocean General Circulation Model (OGCM) for the Earth Simulator 77 (OFES) is considered in this study as the true state of the ocean. The simu-78 lation data is described in Masumoto et al. (2004); Sasaki et al. (2008). The 79 coverage of the model is 75° S- 75° N with a horizontal resolution of $1/10^{\circ}$. 34 80 years (1979-2012) of 3-daily simulation of SSH maps are considered, we pro-81 ceed to a subtraction of a temporal mean to obtain SLA fields. In this study, 82 our region of interest is located in the South China Sea (105°E to 117°E, 5°N 83 to 25°N). This dataset is split into a training dataset corresponding to the 84 first 33 years (4017 SLA maps) and a test dataset corresponding to the last 85 year of the time series (122 SLA maps). 86

87 2.2. Along track data

We consider a realistic situation with a high rate of along track data. More precisely we use along-track data positions registered in 2014 where 4 satellites (Jason2, Cryosat2, Saral/AltiKa, HY-2A) were operating. Data is distributed by Copernicus Marine and Environment Monitoring Service (CMEMS).

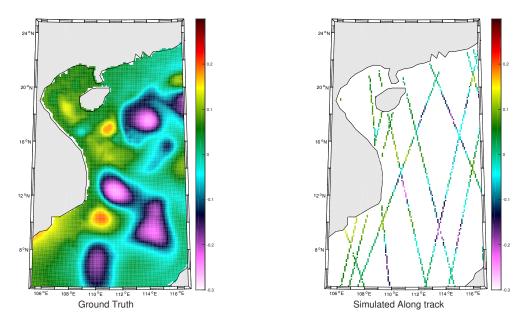


Figure 1: An example of a ground-truth SLA field in the considered region and its associated simulated pseudo-along track.

From the reference 3-daily SLA dataset and real along-track data posi-93 tions, we generate simulated along-track data from the sampling of a ref-94 erence SLA field: more precisely, for a given along-track point, we sample 95 the closest position of the $1/10^{\circ}$ regular model grid at the closest time step 96 of the 3-daily model time series. As we consider a 3-daily assimilation time 97 step (see Section 2.1 for details), we create a 3-daily pseudo-observation field, 98 to be fed directly to the assimilation model. As sketched in Figure 2, for a 99 given time t, we combine all along-track positions for times t - 1, t and t + 1100 to create an along-track pseudo-observation field at time t. We denote by 101 s3dAT the simulated 3-daily time series of along-track pseudo-observation 102 fields. An example of these fields is given in Figure 1. 103

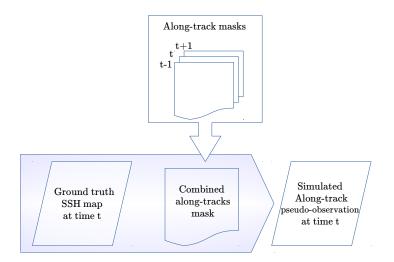


Figure 2: Sketch of the creation of simulated along-track data at a given time t

¹⁰⁴ 3. Problem statement and related work

¹⁰⁵ 3.1. Data assimilation and optimal interpolation

Data assimilation consists in estimating the true state of a physical vari-106 able $\mathbf{x}(t)$ at a specific time t, by combining i) equations governing the dynam-107 ics of the variable, ii) available observations $\mathbf{y}(1,..,T)$ measuring the variable 108 and iii) a background or first guess on its initial state \mathbf{x}^{b} . The estimated state 109 is generally called the analyzed state and noted by \mathbf{x}^{a} . Data assimilation is 110 a typical example of inverse problems, and similar formulations are known 111 to the statistical signal processing community through optimal control and 112 estimation theory (Bocquet et al., 2010). We adopt here the unified notation 113 of Ide et al. (1997) and formulate the problem as a stochastic system in the 114 following: 115

$$\int \mathbf{x}(t) = \mathcal{M}(\mathbf{x}(t-1)) + \eta(t), \tag{1}$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t)) + \epsilon(t).$$
(2)

Equation 1 represents the dynamical model governing the evolution of state 116 **x** through time, while η is a Gaussian centered noise of covariance **Q** that 117 models the process error. Equation 2 explains the relationship between the 118 observation $\mathbf{y}(t)$ and the state to be estimated $\mathbf{x}(t)$ through the operator 119 \mathcal{H} . The uncertainty of the observation model is represented by the ϵ error, 120 considered here to be Gaussian centered and of covariance **R**. We assume that 121 ϵ and η are independent and that Q and R are known. Two main approaches 122 are generally considered for the mathematical resolution of the system (1)-123 (2), namely, variational data assimilation and stochastic data assimilation. 124 They differ in the way they infer the analyzed state x^a , the first is based on 125 the minimization of a certain cost function while the latter aims to obtain 126 an optimal a posteriori estimate. We encourage the reader to consider the 127 book of Asch et al. (2016) for detailed insights on the various aspects and 128 methods of data assimilation. 129

A popular data assimilation algorithm that is largely used in the literature 130 to grid sea level anomalies from along-track data is called Optimal Interpo-131 lation (OI) (e.g. Le Traon et al. (1998); De Mey and Robinson (1987)), this 132 algorithm is also the method adopted in CMEMS altimetry product. Opti-133 mal Interpolation (OI) aims at finding the Best Linear Unbiased Estimator 134 (BLUE) of a field \mathbf{x} given irregularly sampled observations \mathbf{y} in space and 135 time and a background prior \mathbf{x}^{b} . The multivariate OI equations were derived 136 in Gandin (1966) for meteorology and numerous applications in oceanog-137 raphy have been reported since the early work of Bretherton et al. (1976). 138

¹³⁹ Supposing that the background state \mathbf{x}^{b} has covariance B, and the observa-¹⁴⁰ tion operator is linear $\mathcal{H} = \mathbf{H}$, the analyzed state \mathbf{x}^{a} and the analyzed error ¹⁴¹ covariance \mathbf{P}^{a} can be calculated using the following OI set of equations:

$$\mathbf{K} = \mathbf{B}\mathbf{H}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}$$
 called the Kalman gain (3)

$$\mathbf{x}^{a} = \mathbf{x}^{b} + \mathbf{K}(\mathbf{y} - \mathbf{H}\mathbf{x}^{b}) \tag{4}$$

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{B} \tag{5}$$

It worths mentioning that Lorenc (1986) showed that OI is closely related to the 3D-Var variational data assimilation algorithm which obtains \mathbf{x}^{a} by minimizing the following cost function:

$$J(x) = (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + (\mathbf{y} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}\mathbf{x})$$
(6)

While OI had been shown to successfully retrieve large-scale structures in the ocean ($\geq 150 km$), a well-known limitation of OI is that the Gaussianlike covariance error matrices smooths out the small-scale information (*e.g.* mesoscale eddies) (Ubelmann et al., 2014). OI would then underexploit high resolution altimeter data in the context of future altimetry missions, which urges to put efforts in trying to improve the method (e.g. Escudier et al. (2013a)) or find other alternatives.

152 3.2. Analog data assimilation

Endorsed by the recent development in data-driven methods and data storage capacities, the Analog Data Assimilation (AnDA) was introduced as an alternative to classical model-driven data assimilation under one or more of the following situations (Lguensat et al., 2017): • The model is inconsistent with observations

• The cost of the model integration is high computationally

• (mandatory) The availability of large datasets of past dynamics of the variables to be estimated. These datasets are hereinafter called catalogs and denoted by C. The catalog is organized in a two-column dictionary where each state of the system is associated with its successor in time, forming a set of couples $(\mathcal{A}_i, \mathcal{S}_i)$ where \mathcal{A}_i is called the *analog* and \mathcal{S}_i its *successor*.

Given the considerations above, AnDA resorts to evaluating filtering, resp. smoothing, posterior likelihood, *i.e.* the distribution of the state to be estimated $\mathbf{x}(t)$ at time t, given past and current observations $\mathbf{y}(1,..,t)$, resp. given all the available observation $\mathbf{y}(1,..,T)$. This evaluation relies on the following state-space model:

$$\begin{cases} \mathbf{x}(t) = \mathcal{F}(\mathbf{x}(t-1)) + \eta(t), \tag{7} \end{cases}$$

$$\mathbf{y}(t) = \mathcal{H}(\mathbf{x}(t)) + \epsilon(t). \tag{8}$$

The difference between AnDA and classical data assimilation resides in 170 the transition model equation 7. The counterpart of a model-driven operator 171 \mathcal{M} of Equation 1 is here the operator \mathcal{F} which refers to the considered data-172 driven operator, so called, the analog forecasting operator. This operator 173 makes use of the available catalog \mathcal{C} and assumes that the state forecast can 174 be inferred from similar situations in the past. Provided the definitions of the 175 analogs and successors given above, the derivation of this operator resorts 176 to characterizing the transition distribution *i.e.* $p(\mathbf{x}(t)|\mathbf{x}(t-1))$. Following 177 Lguensat et al. (2017), a Gaussian conditional distribution is adopted: 178

$$\mathbf{x}(t)|\mathbf{x}(t-1) \sim \mathcal{N}(\mu_t, \Sigma_t) \tag{9}$$

where $\mathcal{N}(\mu_t, \Sigma_t)$ is a Gaussian distribution of mean μ_t and covariance Σ_t . These parameters of the Gaussian distribution are calculated using the result of a K nearest neighbors search. The K nearest neighbors (analogs) $\mathcal{A}_{k \in (1,..,K)}$ of state $\mathbf{x}(t-1)$ and their successors $\mathcal{S}_{k \in (1,..,K)}$, along with a weight associated to each pair $(\mathcal{A}_k, \mathcal{S}_k)$ are used to calculate μ_t and Σ_t , the forecast state $\mathbf{x}(t)$ is then sampled from $\mathcal{N}(\mu_t, \Sigma_t)$. The weights are defined using a Gaussian kernel \mathcal{K}_G .

$$\mathcal{K}_G(u,v) = \exp\left(-\frac{\|u-v\|^2}{\sigma}\right),\tag{10}$$

Scale parameter σ is locally-adapted to the median value of the K distances $\|x(t-1) - \mathcal{A}_k\|^2$ to the K analogs. Other types of kernels might be considered (e.g. Zhao and Giannakis (2014b); McDermott and Wikle (2015)), investigating kernel choice is out of the scope of this paper.

The mean and the covariance of the transition distribution might be calculated following several strategies. We consider in this work the three analog forecasting operators introduced in AnDA (Lguensat et al., 2017):

- Locally-constant operator: Mean μ_t and covariance Σ_t are given by the weighted mean and covariance of the K successors $S_{k \in (1,..,K)}$.
- Locally-incremental operator: Here, the increments between the Kanalogs and their corresponding successors are calculated $S_{k \in (1,..,K)}$ – $\mathcal{A}_{k \in (1,..,K)}$. The weighted mean of the K increments is then added to

the $\mathbf{x}(t-1)$ to obtain μ_t . While Σ_t results in the weighted covariance of these differences.

• Locally-linear operator: A weighted least-square estimation of the linear regression of the state at time t given the state at time t - 1 is performed based on the K pairs $(\mathcal{A}_k, \mathcal{S}_k)$. The parameters of the linear regression are then applied to state $\mathbf{x}(t-1)$ to obtain μ_t . Covariance Σ_t is represented by the covariance of the residuals of the fitted weighted linear regression.

The application of the AnDA framework faces the curse of dimensionality 206 the search of analogs is highly affected by the dimensionality of the i.e. 207 problem and can be irrelevant for dimensions above 20 (Lguensat et al., 208 2017). As proposed in Fablet et al. (2017), the extension of AnDA models to 209 high-dimensional fields may then rely on turning the global assimilation issue 210 into a series of lower-dimensional ones. We consider here an approach similar 211 to Fablet et al. (2017) using a patch-based and EOF-based representation of 212 the 2D fields, *i.e.* the 2D fields are decomposed into a set of overlapping 213 patches, each patch being projected onto an EOF space. Analog strategies 214 then apply to patch-level time series in the EOF space. 215

Overall, as detailed in the following section, the proposed analog data assimilation model for SLA fields relies on three key components: a patchbased representation of the SLA fields, the selection of a kernel to retrieve analogs and the specification of a patch-level analog forecasting operator.

220 4. Analog reconstruction for altimeter-derived SLA

221 4.1. Patch-based state-space formulation

As stated above, OI may be considered as an efficient model-based method to recover large-scale structures of SLA fields. Following Fablet et al. (2017), this suggests considering the following two-scale additive decomposition:

$$X = \bar{X} + dX + \xi \tag{11}$$

where \bar{X} is the large-scale component of the SLA field, typically issued from an optimal interpolation, dX the fine-scale component of the SLA field we aim to reconstruct and ξ remaining unresolved scales.

The reconstruction of field dX involves a patch-based and EOF-based 228 representation. It consists in regarding field dX as a set of $P \times P$ overlap-229 ping patches (e.g. $2^{\circ} \times 2^{\circ}$). This set of patches is referred to as \mathcal{P} , and we 230 denote by \mathcal{P}_s the patch centered on position s. After building a catalog $\mathcal{C}_{\mathcal{P}}$ 231 of patches from the available dataset of residual fields $X - \bar{X}$ (see Section 232 3.2), we proceed to an EOF decomposition of each patch in the catalog. The 233 reconstruction of field $dX(\mathcal{P}_s, t)$ at time t is then stated as the analog assim-234 ilation of the coefficients of the EOF decomposition in the EOF space given 235 an observation series in the patch space. Formally, $dX(\mathcal{P}_s, t)$ decomposes as 236 a linear combination of a number N_E of EOF basis functions: 237

$$dX(\mathcal{P}_s, t) = \sum_{k=1}^{N_E} \alpha_k(s, t) EOF_k$$
(12)

with EOF_k the k^{th} EOF basis and $\alpha_k(s, t)$ the corresponding coefficient for patch \mathcal{P}_s at time t. Let us denote by $\Phi(\mathcal{P}_s, t)$ the vector of the N_E coefficients ²⁴⁰ $\alpha_k(s,t)$. This vector represents the projection of $dX(\mathcal{P}_s,t)$ in the lower-²⁴¹ dimensional EOF space.

242 4.2. Patch-based analog dynamical models

Given the considered patch-based representation of field dX, the proposed patch-based analog assimilation scheme involves a dynamical model stated in the EOF space. Formally, Equation 9 leads to the following Gaussian conditional distribution in the EOF space

$$\Phi(\mathcal{P}_s, t) | \Phi(\mathcal{P}_s, t-1) \sim \mathcal{N}(\mu(s, t), \Sigma(s, t))$$
(13)

We consider the three analog forecasting operators presented in Section 3.2, 247 namely, the locally-constant, the locally incremental and the locally-linear. 248 The calculation of the weights associated to each analog-successor pair relies 249 on a Gaussian kernel \mathcal{K}_G (Equation 10). The search for analogs in the N_E -250 dimensional patch space (in practice, N_E ranges from 5 to 20) ensures a better 251 accuracy in the retrieval of relevant analogs compared to a direct search in 252 the high-dimensional space of state dX. It also reduces the computational 253 complexity of the proposed scheme. 254

Another important extension of the current study is the possibility of exploiting auxiliary variables with the state vector Φ in the analog forecasting models. Such variables may be considered in the search for analogs as well as regression variables in locally-linear analog setting. Regarding the targeted application to the reconstruction of SSH fields and the proposed two-scale decomposition (Equation 11), two types of auxiliary variables seem to be of interest: the low-resolution component \bar{X} to take into account inter-scale relationship (Fablet et al., 2016), and Sea Surface Temperature (SST) with
respect to the widely acknowledged SST-SSH synergies (Fablet et al., 2016;
Klein et al., 2009; Isern-Fontanet et al., 2014). We also apply patch-level
EOF-based decompositions to include both types of variables in the considered analog forecasting models (Equation 13).

267 4.3. Numerical resolution

Given the proposed analog assimilation model, the proposed scheme first 268 relies on the creation of patch-level catalogs from the training dataset. This 260 step requires the computation of a training dataset of fine scale data $dX_{training}$, 270 this is done by subtracting a large-scale component $X_{training}$ from the origi-271 nal training dataset. Here, we consider the large-scale component of training 272 data to be the result of a global¹ EOF-based reconstruction using a number 273 of EOF components that retains 95% of the dataset variance, which accounts 274 for horizontal scales up to ~ 100 km. This global EOF-based decomposition 275 provides a computationally-efficient means for defining large-scale component 276 \bar{X} . This EOF-based decomposition step is followed by the extraction of over-277 lapping patches for all variables of interest, namely $\bar{X}_{training}$, $dX_{training}$ and 278 potential auxiliary variables, and the identification of the EOF basis func-279 tions from the resulting raw patch datasets. This leads to the creation of a 280 patch-level catalog $\mathcal{C}_{\mathcal{P}}$ from the EOF-based representations of each patch. 281

Given the patch-level catalog, the algorithm applied for the mapping SLA fields from along-track data, referred to PB-AnDA (for Patch-Based AnDA),

¹By global, we mean here an EOF decomposition over the entire case study region, by contrast to the patch-level decomposition considered in the analog assimilation setting.

²⁸⁴ involves the following steps:

- the computation of the large-scale component \bar{X} , here, we consider the result of optimal interpolation (OI) projected onto the global EOF basis functions.
- 288

289

• the decomposition of the case study region into overlapping $P \times P$ patches, here, 20 × 20 patches

• For each patch position s, the application of an analog data assimilation 290 scheme, namely the Analog Ensemble Kalman Smoother (AnEnKS) 291 (Lguensat et al., 2017), for patch \mathcal{P}_s of field dX. As stated in (13), the 292 assimilation is performed in the EOF space, *i.e.* for EOF decomposition 293 $\Phi(\mathcal{P}_s, t)$, using the operator derived from EOF-based reconstruction 294 (12) and decomposition (11) as observation model \mathcal{H} in (8) and the 295 patch-level training catalog described in the previous section. In the 296 analog forecasting setting, The search for analogs is restricted to patch 297 exemplars in the catalog within a local spatial neighborhood (typically 298 a patch-level 8-neighborhood), except for patches along the seashore 299 for which the search for analogs is restricted to patch exemplars at the 300 same location. 301

• the reconstruction of fields dX from the set of assimilated patches $\{dX(\mathcal{P}_s, \cdot)\}_s$. This relies on a spatial averaging over overlapping patches (here, a 5-pixel overlapping in both directions). In practice, we do not apply the patch-level assimilation to all grid positions. Consequently, the spatial averaging may result in blocky artifacts. We then apply

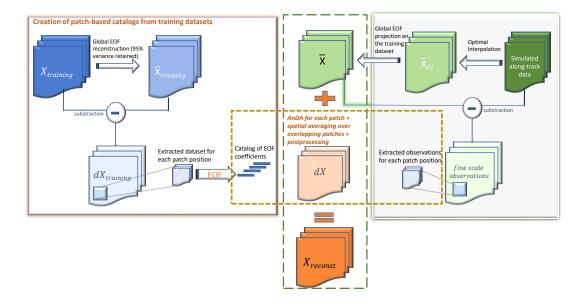


Figure 3: Sketch of the proposed patch-based Analog Data Assimilation (PB-AnDA). The left block details the construction of the patch-based catalogs from the training dataset. The right block illustrates the process of obtaining the large-scale component of the SLA reconstructed field. The orange dashed rectangle represents the application of the AnDA using the catalog and the fine-scale observations. Finally, the green dashed rectangle shows the final addition operation that yields the reconstructed SLA field.

a patchwise EOF-based decomposition-reconstruction with a smaller patch-size (here, 17×17 patches) to remove these blocky artifacts.

• the reconstruction of fields X as $\overline{X} + dX$.

310 5. Results

We evaluate the proposed PB-AnDA approach using the OSSE presented in Section 2. We perform a qualitative and quantitative comparison to stateof-the-art approaches. We first describe the parameter setting used for the PB-AnDA as well as benchmarked models, namely OI, an EOF-based approach (Ping et al., 2016) and a direct application of AnDA at the region level. We then report numerical experiments for noise-free and noisy observation data as well the relevance of auxiliary variables in the proposed PB-AnDA scheme.

319 5.1. Experimental setting

We detail below the parameter setting of the models evaluated in the reported experiments, including the proposed PB-AnDA scheme:

• *PB-AnDA*: We consider 20×20 patches with 15-dimensional EOF de-322 compositions $(N_E = 15)$, which typically accounts for 99% of the data 323 variance for the considered dataset. The postprocessing step exploits 324 17×17 patches and a 15-dimensional EOF decomposition. Regard-325 ing the parametrization of the AnEnKS procedure, we experimentally 326 cross-validated the number of nearest neighbors K to 50, the number 327 of ensemble members $n_{ensemble}$ to 100 and the observation covariance 328 error in Equation 8 to $\mathbf{R} = 0.001$. 329

• Optimal Interpolation: We apply an Optimal Interpolation to the processed along-track data. It provides the low-resolution component for the proposed PB-AnDA model and a model-driven reference for evaluation purposes. The background field is a null field. We use a Gaussian covariance model with a spatial correlation length of 100km and a temporal correlation length of 15 days (\pm 5 timesteps since our data is 3-daily). These choices result from a cross-validation experiment.

• *VE-DINEOF*: We apply a second state-of-the-art interpolation scheme 337 using a data-driven strategy solely based on EOF decompositions, namely 338 VE-DINEOF (Ping et al., 2016). We implement a patch-based version 339 of VE-DINEOF to make it comparable to the proposed PB-AnDA set-340 ting. Given the same EOF decomposition as in PB-AnDA, the patch-341 level VE-DINEOF iterates patchwise EOF projection-reconstruction 342 of the detail field dX. This scheme is initialized from the along-track 343 pseudo-observation field for along-track data positions and \overline{X} for miss-344 ing data positions. After each projection-reconstruction, we only up-345 date missing data areas. We run this iterative process until conver-346 gence. 347

• G-AnDA: With a view to evaluating the relevance of the patch-based 348 decomposition, we also apply AnDA at the region scale, referred to as 349 G-AnDA. It relies on an EOF-based decomposition of the detail field 350 dX. We use 150 EOF components, which accounts for more than 99% 351 of the total variance of the SSH dataset. From cross-validation ex-352 periments, the associated AnEnKS procedure relies on a locally-linear 353 analog forecasting model with K = 500 analogs, $n_{ensemble} = 100$ en-354 semble members and an observation covariance error in Equation 8 set 355 to $\mathbf{R} = 0.001$ 356

The patch-based experiments were run on Teralab infrastructure using a multi-core virtual machine (30 CPUs, 64G of RAM). We used the Python toolbox for patch-based analog data assimilation (Fablet et al., 2017) (available at github.com/rfablet/PB_ANDA). Optimal Interpolation was implemented on Matlab using Escudier et al. (2013b). Throughout the experiments, two metrics are used to assess the performance of the considered interpolation methods: i) daily and mean Root Mean Square Error (RMSE) series between the reconstructed SLA fields X and the groundtruthed ones, ii) daily and mean correlation coefficient between the fine-scale component dX of the reconstructed SLA fields and of the groundtruthed ones.

367 5.2. SLA reconstruction from noise-free along-track data

We first perform an idealized noise-free experiment, where the along-track 368 observations are noise-free. The observation covariance error in Equation 8 360 takes the value $\mathbf{R} = 0.001$. The interpolation performances for this ex-370 periment are illustrated in Table 1. Our PB-AnDA algorithm significantly 371 outperforms OI. More specifically, the locally-linear PB-AnDA results in the 372 best reconstruction among the competing methods. We suggest that this im-373 provement comes from the reconstruction of fine-scale features learned from 374 the archived model simulation data. Figure 4a reports interpolated SSH fields 375 and their gradient fields which further confirm our intuition. PB-AnDA in-376 terpolation shows an enhancement of the gradients and comes out with some 377 fine-scale eddies that were smoothed out in OI and VE-DINEOF. This is also 378 confirmed by the Fourier power spectrum of the interpolated SLA fields in 379 Figure 4b. 380

Table 1: SLA Interpolation performance for a noise-free experiment: Root Mean Square Error (RMSE) and correlation statistics for OI, VE-DINEOF, G-AnDA and PB-AnDA w.r.t. the groundtruthed SLA fields. See Section 5.1 for the corresponding parameter settings.

C	Criterion	RMSE	Correlation	
OI		0.026 ± 0.007	0.81 ± 0.08	
VE-DINEOF		0.023 ± 0.007	0.85 ± 0.07	
G-AnDA		0.020 ± 0.006	0.89 ± 0.04	
PB-AnDA	Locally-constant	0.014 ± 0.005	0.95 ± 0.03	
	Locally-Increment	0.014 ± 0.005	0.95 ± 0.03	
	Locally-Linear	0.013 ± 0.005	0.96 ± 0.02	

381 5.3. SLA reconstruction from noisy along-track data

We also evaluated the proposed approach for noisy along-track data. Here, we run two experiments with an additive zero-mean Gaussian noise applied to the simulated along-track data. We consider a noise covariance of $\mathbf{R} = 0.01$ (Experiment A) and of $\mathbf{R} = 0.03$ (Experiment B) which is more close to the instrumental error of conventional altimeters. Given the resulting noisy along-track dataset, we apply the same methods as for the noise-free case study.

We run PB-AnDA using different values for **R**. For Experiment A, Table 2 shows that the minimum is reached using the true value of the error $\mathbf{R} =$ 391 0.01. While for Experiment B, Table 3 shows that the minimum is counter-

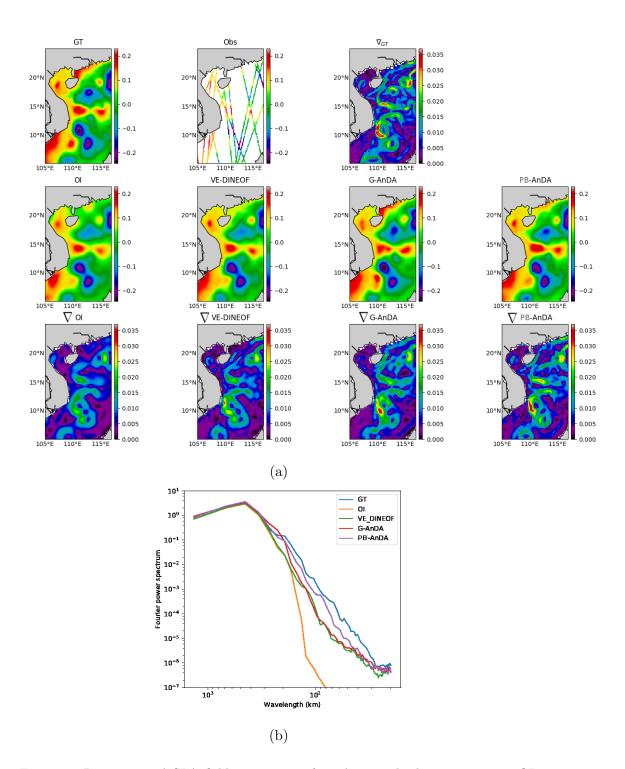


Figure 4: Reconstructed SLA fields using noise-free along-track observation using OI, DINEOF, G-AnDA, PB-AnDA on the $54^{th}22ay$ (February 24^{th} 2012): from left to right, the first row shows the ground truth field, the simulated available along-tracks for that day, the ground truth gradient field. The second and third rows show each of the reconstruction and their corresponding gradient fields, from left to right, OI, VE-DINEOF, G-ANDA and PB-AnDA. The Fourier power spectrum of the competing methods is also included

³⁹² intuitively reached again using value of the error $\mathbf{R} = 0.01$.

Our algorithm is then compared with the results of the application of the 393 competing algorithms considered in this work. Results are shown in Table 394 4. PB-AnDA still outperforms OI in terms of RMSE and correlation statis-395 tics in both experiments. The locally-linear version of PB-AnDA depicts the 396 best reconstruction performance. We report an example of the reconstruc-397 tion in Figure 5. Similarly to the noise-free case study, PB-AnDA better 398 recovers finer-scale structures in Fig.5.a compared with OI, VE-DINEOF 399 and G-AnDA. In Fig.5.b, PB-AnDA also better reconstructs a larger-scale 400 North-East structure, poorly sampled by along-track data and hence poorly 401 interpolated by OI. 402

Table 2: Impact of variance of observation error R in AnDA interpolation performance using noisy along-track data (R=0.01): RMSE of AnDA interpolation for different values of parameter R. For the same dataset, OI RMSE is **0.039**.

R	0.1	0.05	0.03	0.01	0.005	0.001	0.0001
rmse _{PB-AnDA}	0.035	0.030	0.028	0.025	0.025	0.029	0.044

Table 3: Impact of variance of observation error R in AnDA interpolation performance using noisy along-track data (R=0.03): RMSE of AnDA interpolation for different values of parameter R. For the same dataset, OI RMSE is **0.066**.

R	0.1	0.05	0.03	0.01	0.005	0.001	0.0001
$rmse_{PB-AnDA}$	0.038	0.036	0.035	0.0349	0.037	0.046	0.076

Table 4: SLA Interpolation performance for noisy along-track data: Root Mean Square Error (RMSE) and correlation statistics for OI, VE-DINEOF, G-AnDA and PB-AnDA w.r.t. the groundtruthed SLA fields. See Section 5.1 for the corresponding parameter settings.

	С	riterion	RMSE	Correlation	
R=0.01	OI		0.039 ± 0.005	0.64 ± 0.09	
	VE-DINEOF		0.035 ± 0.005	0.68 ± 0.09	
	G-AnDA		0.030 ± 0.005	0.78 ± 0.06	
		Locally constant	0.026 ± 0.005	0.82 ± 0.05	
	PB-AnDA	Increment	0.028 ± 0.005	0.81 ± 0.05	
		Local Linear	$\textbf{0.0245} \pm \textbf{0.005}$	$\boldsymbol{0.83}\pm\boldsymbol{0.05}$	
R=0.03	OI		0.066 ± 0.006	0.41 ± 0.09	
	VE-DINEOF		0.060 ± 0.006	0.45 ± 0.09	
	G-AnDA		0.039 ± 0.006	0.67 ± 0.09	
		Locally constant	0.035 ± 0.006	0.688 ± 0.064	
	PB-AnDA	Increment	0.036 ± 0.006	0.656 ± 0.07	
		Local Linear	0.032 ± 0.006	0.708 ± 0.063	

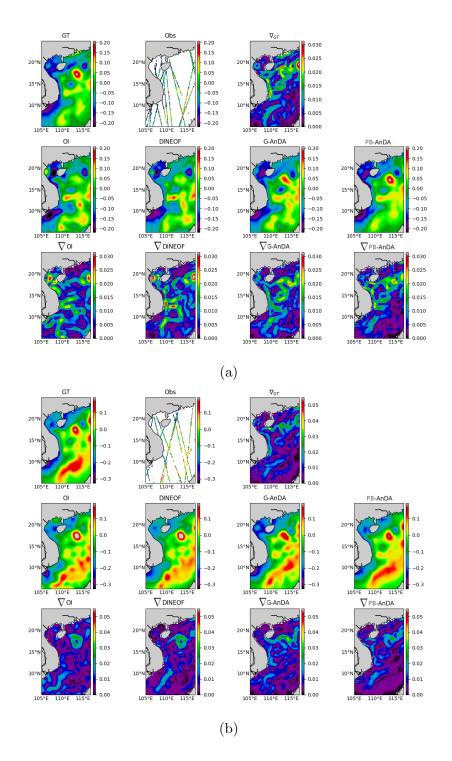


Figure 5: Reconstruction of SLA fields from noisy along-track data using OI, DINEOF, G-AnDA & PB-AnDA on day 225^{th} (a) & 228^{th} (b)

403 5.4. PB-AnDA models with auxiliary variables

We further explore the flexibility of the analog setting to the use of ad-404 ditional geophysical variable information as explained in Section 4.2. In-405 tuitively, we expect SLA fields to involve inter-scale dependencies as well 406 as synergies with other tracers. The use of auxiliary variables provide the 407 means for evaluating such dependencies and their potential impact on recon-408 struction performance. We consider two auxiliary variables that are used in 409 the locally-linear analog forecasting model (7): i) to account for the rela-410 tionship between the large-scale and fine-scale component, we may consider 411 variable \bar{X} , ii) considering potential SST-SSH synergies, we consider SST 412 fields. Overall, we consider four parameterization of the regression variables 413 used in PB-AnDA: the sole use of dX (PB-AnDA-dX); the joint use of dX414 and SST fields (PB-AnDA-dX+SST); the joint use of dX and \bar{X} (PB-AnDA-415 $dX+\bar{X}$), the joint use of dX and the groud ntruthed version of \bar{X} denoted by 416 \bar{X}^{GT} , (PB-AnDA-dX+ \bar{X}^{GT}). The later provides a lower-bound for the recon-417 struction performance, assuming the low-resolution component is perfectly 418 estimated. 419

We report mean RMSE and correlation statistics for these four PB-420 AnDA parameterizations in Table 5 for the noisy case-study. Considering 421 PB-AnDA-dX as reference, these results show a very slight improvement 422 when complementing dX with SST information. Though limited, we report 423 a greater improvement when adding the low-resolution component X. In-424 terestingly, a significantly greater improvement is obtained when adding the 425 true low-resolution information. The mean results are in accordance with 426 Fablet et al. (2016), which reported that large-scale SLA information was 427

⁴²⁸ more informative than SST to improve the reconstruction of the SLA at ⁴²⁹ finer scales. Though mean statistics over one year leads to rather limited ⁴³⁰ improvement, daily RMSE time series (Figure 6) reveal that for some peri-⁴³¹ ods, for instance between day 130 and 150, relative improvements in terms ⁴³² of RMSE may reach 10% with the additional information brought by the ⁴³³ large-scale component. In this respect, it may noted that PB-AnDA-dX+ \bar{X} ⁴³⁴ always perform better than PB-AnDA-dX.

Table 5: PB-AnDA reconstruction performance using noisy along-track data for different choices of the regression variables in the locally-linear analog forecasting model: PB-AnDA-dX using solely dX, PB-AnDA-dX+SST using both dX and SST, PB-AnDA- $dX+\bar{X}$ using both dX and \bar{X} , and PB-AnDA- $dX+\bar{X}^{GT}$ using dX and the true large-scale component \bar{X}^{GT} .

	PB-AnDA model	RMSE	Correlation	
R = 0.01	PB-AnDA- dX	0.025 ± 0.005	0.83 ± 0.05	
	PB-AnDA- dX +SST	0.024 ± 0.005	0.83 ± 0.05	
	PB-AnDA- $dX + \bar{X}$	0.023 ± 0.005	0.84 ± 0.05	
	PB-AnDA- $dX + \bar{X}^{GT}$	0.021 ± 0.004	0.87 ± 0.04	
R=0.03	PB-AnDA-dX	0.032 ± 0.006	0.708 ± 0.06	
	$\operatorname{PB-AnDA-}dX + \operatorname{SST}$	0.031 ± 0.006	0.710 ± 0.06	
	PB-AnDA- $dX + \bar{X}$	0.029 ± 0.006	0.717 ± 0.06	
_	PB-AnDA- $dX + \bar{X}^{GT}$	0.026 ± 0.005	0.730 ± 0.05	

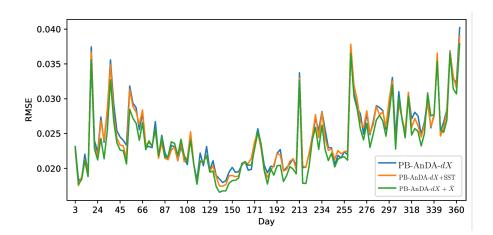


Figure 6: Daily RMSE time series of PB-AnDA SLA reconstructions using noisy along-track data for different choices of the regression variables in the locally-linear analog fore-casting model: PB-AnDA-dX (light blue), PB-AnDA-dX+SST (orange) and PB-AnDA- $dX + \bar{X}$ (green).

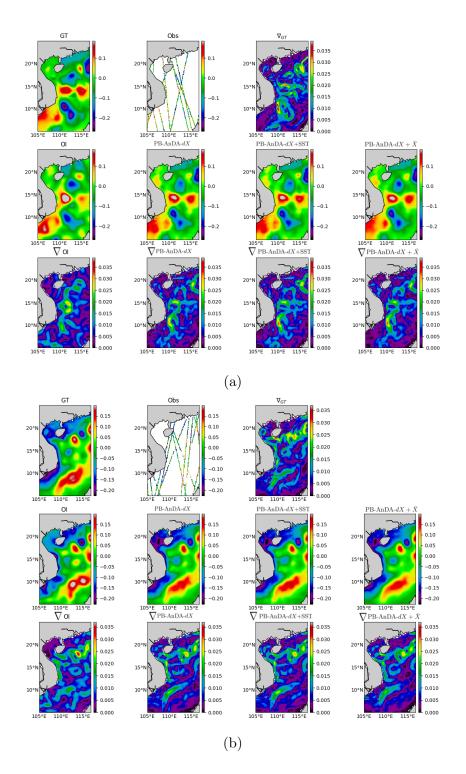


Figure 7: (Noisy observation) Reconstruction of SLA fields using PB-AnDA with different multivariate regression models on day $57^{th} \& 237^{th}$ (b)

435 6. Discussion and conclusion

This work sheds light on the opportunities that data science methods are 436 offering to improve altimetry in the era of "Big Data". Assuming the avail-437 ability of high-resolution numerical simulations, we show that Analog Data 438 Assimilation (AnDA) can outperform the Optimal Interpolation method and 430 retrieve smoothed out structures resulting from the sole use of OI both with 440 idealized noise-free and more realistic noisy observations for the considered 441 case study. Importantly, the reported experiments point out the relevance for 442 combining OI for larger scales (above 100km) whereas the proposed patch-443 based analog setting successfully applies to the finer-scale range below 100km. 444 This is in agreement with the recent application of the analog data assimila-445 tion to the reconstruction of cloud-free SST fields (Fablet et al., 2017). We 446 also demonstrate that AnDA can embed complementary variables in a sim-447 ple manner through the regression variables used in the locally-linear analog 448 forecasting operator. In agreement with our recent analysis (Fablet et al., 449 2016), we demonstrate that the additional use of local SST and large-scale 450 SLA information may further improve the reconstruction performance for 451 fine-scale structures. 452

Analog data assimilation can be regarded as a means to fuse ocean models and satellite-derived data. We regard this study as a proof-of-concept, which opens research avenues as well as new directions for operational oceanography. Our results advocate for complementary experiments at the global scale or in different ocean regions for a variety of dynamical situations with a view to further evaluating the relevance of the proposed analog assimilation framework. Such experiments should evaluate the sensitivity of the assimilation

with respect to the size of the catalog. The scaling up to the global ocean also 460 suggests investigating computationally-efficient implementation of the ana-461 log data assimilation. In this respect, the proposed patch-based framework 462 intrinsically ensures high parallelization performance. From a methodolog-463 ical point of view, a relative weakness of the analog forecasting models (9) 464 may be their low physical interpretation compared with physically-derived 465 priors (Ubelmann et al., 2014). The combination of such physically-derived 466 parameterizations to data-driven strategies appear as a promising research 467 direction. 468

Beyond along-track altimeter data as considered in this study, future 469 missions such as SWOT (NASA/CNES) promise an unprecedented coverage 470 around the globe. More specifically, the large swath is expected to provide a 471 large number of data, urging for the inspection of the potential improvements 472 that this new mission will bring compared to classical along-track data. In 473 the context of analog data assimilation, the interest of SWOT data may be 474 two-fold. First, regarding observation model (8), SWOT mission will both 475 significantly increase the number of available observation data and enable 476 the definition of more complex observation models exploiting for instance 477 velocity-based or vorticity-based criterion. Second, SWOT data might also 478 be used to build representative patch-level catalogs of exemplars. Future 479 work should investigate these two directions using simulated SWOT test-480 beds (Gaultier et al., 2015). 481

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