

1 **Unsupervised Learning of Sea Surface Height**
2 **Interpolation from Multi-variate Simulated Satellite**
3 **Observations.**

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10 **Key Points:**

- 11 • This is the preprint of a paper submitted to JAMES in September 2023
- 12 • We developed a realistic simulation of satellite observations of sea surface height
- 13 and temperature
- 14 • We compare deep learning supervised and unsupervised strategies to interpolate
- 15 the sea surface height, and able to use temperature data
- 16 • We find temperature, enhances sea surface height reconstruction, as well as the
- 17 estimation of the surface currents and mesoscale eddies.

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Abstract

Satellite-based remote sensing missions have revolutionized our understanding of the Ocean state and dynamics. Among them, spaceborne altimetry provides valuable measurements of Sea Surface Height (SSH), which is used to estimate surface geostrophic currents. However, due to the sensor technology employed, important gaps occur in SSH observations. Complete SSH maps are produced by the altimetry community using linear Optimal Interpolations (OI) such as the widely-used Data Unification and Altimeter Combination System (DUACS). However, OI is known for producing overly smooth fields and thus misses some mesostructures and eddies. On the other hand, Sea Surface Temperature (SST) products have much higher data coverage and SST is physically linked to geostrophic currents through advection. We design a realistic twin experiment to emulate the satellite observations of SSH and SST to evaluate interpolation methods. We introduce a deep learning network able to use SST information, and a trainable in two settings: one where we have no access to ground truth during training and one where it is accessible. Our investigation involves a comparative analysis of the aforementioned network when trained using either supervised or unsupervised loss functions. We assess the quality of SSH reconstructions and further evaluate the network's performance in terms of eddy detection and physical properties. We find that it is possible, even in an unsupervised setting to use SST to improve reconstruction performance compared to SST-agnostic interpolations. We compare our reconstructions to DUACS's and report a decrease of 41% in terms of root mean squared error.

Plain Language Summary

The surface of the ocean is observed through various sensors embedded in satellites. Specifically, the height of the sea surface is a very important variable as it can be used to estimate surface currents. It is currently measured through satellite altimeters, but the data acquisition process leaves gaps in their observations. Providing fully gridded maps of the sea surface height is thus an important interpolation problem. The widely used interpolated product has some troubles especially when dealing with small and rapidly evolving eddies. To enhance the quality of the height map, we propose to use an artificial neural network, a trainable method able to estimate complete sea surface height images. The flexibility of these methods allows us to use different satellite information, such as the sea surface temperature, which is acquired with a much better resolution. Usually, neural networks are trained on a dataset upon which they learn the link between input and output data. However in a realistic geoscience scenario, the output is never known for sure, so we propose a methodology to train these methods using only the input information. We show the feasibility of these approaches, as well as the improvements brought by the temperature information.

1 Introduction

Since the first ocean remote sensing missions in the 1970s, satellite observation of the ocean has become one of the most determining contributions to understanding ocean state and dynamics (S. Martin, 2014). Through the years, satellites have provided a huge amount of measures of various physical natures with wide spatial coverage that completed in situ datasets. Among these techniques, satellite altimetry is used to retrieve the Sea Surface Height (SSH) a determining variable of the ocean circulation. Indeed, SSH spatial gradient can be used to estimate geostrophic currents, i.e. the currents necessary for the Coriolis force to balance the pressure force in the surface layer of the Ocean. SSH (also called Absolute Dynamical Topography by the altimetry community) is currently measured by nadir-pointing altimeters, meaning that they can only take measurements vertically, along their ground tracks, by calculating the return time of a radar pulse. This leads to important gaps in the observed SSH, and providing a gap-free product (L4) is

68 a challenging Spatio-Temporal interpolation problem. One of the most widely used L4
69 products in oceanography applications is the Data Unification and Altimeter Combina-
70 tion System (DUACS) (Taburet et al., 2019) which performs a linear Optimal Interpo-
71 lation (OI) of the nadir along-track measures leveraging a covariance matrix tuned on
72 25 years of data. However several studies show that DUACS reconstruction misses some
73 of the mesoscales structures and eddies (Amores et al., 2018; Stegner et al., 2021). As
74 such, improving the reconstruction of a gridded altimetry product is still an open chal-
75 lenge.

76 In order to enhance the quality of the SSH reconstruction and sea surface current
77 estimation, using additional physical information such as the Sea Surface Temperature
78 (SST) has been demonstrated to be beneficial (Ciani et al., 2020; Thiria et al., 2023; S. A. Mar-
79 tin et al., 2023; Archambault et al., 2023; Fablet et al., 2023). SST motion is linked to
80 ocean circulation (Isern-Fontanet et al., 2006), and therefore to SSH, as heat is trans-
81 ported by currents in an advection dynamic. SST measurements obtained through pas-
82 sive infrared technology offer a remarkably high spatial resolution, ranging from 1.1 to
83 4.4 km (Emery et al., 1989), even if intermittent cloud coverage also introduces data gaps.
84 Thus, a crucial challenge lies in developing efficient reconstruction methods capable of
85 fusing data derived from different remote sensing techniques, each presenting distinct in-
86 terpolation challenges, thereby unlocking the full potential of satellite oceanography prod-
87 ucts.

88 In the last decade, deep learning has emerged as one of the leading methods in com-
89 puter vision, particularly to address image inverse problems. Neural networks have demon-
90 strated remarkable flexibility in fusing observations from various sources and modalities,
91 exhibiting their capacity to learn complex relationships given a sufficient number of train-
92 ing samples (McCann et al., 2017; Ongie et al., 2020). Prior work proved that it is pos-
93 sible to use SST to enhance SSH reconstruction with a deep-learning network, whether
94 from a downscaling perspective (Nardelli et al., 2022; Thiria et al., 2023) or an interpo-
95 lation one (Fablet et al., 2023; S. A. Martin et al., 2023) However, training such meth-
96 ods often requires the fully gridded ground truth to be trained, which is not possible in
97 a realistic geoscientific scenario. To overcome this limitation two solutions were proposed:
98 employing loss functions that do not rely on ground truth data or conducting a twin ex-
99 periment on a simulation mimicking the inverse problem we try to solve (also called an
100 Observing System Simulation Experiment). This last option has the advantage of allow-
101 ing supervised training but suffers from the domain gap that might occur between the
102 simulation and the real world. Notably, Fablet et al. (2021) performed an efficient su-
103 pervised SSH interpolation on one year of OSSE data and extended their study using
104 SST showing increased performance (Fablet et al., 2023). On the other hand, Archambault
105 et al. (2023); S. A. Martin et al. (2023) trained a neural network using only observations.

106 However, as both these studies focused on real-world data, no fully gridded ground
107 truth reference was available for an evaluation and interpretation of the results. In this
108 work, we design a new OSSE framework including 20 years of SSH and SST simulated
109 observations and their associated ground truth. As the previously existing OSSE (CLS/MEOM,
110 2020) provided only one year of data and no SST realistic instrumental error, this new
111 dataset is closer to a realistic multi-variate observation of the ocean. Moreover, we present
112 a novel Attention-Based Encoder-Decoder (ABED) framework to perform spatiotempo-
113 ral interpolation of SSH fields. This network leverages along-track SSH measurements
114 and, optionally, incorporates SST contextual data. In order to assess the feasibility of
115 training ABED in a realistic setting, where no gridded ground truth is accessible, we pro-
116 pose to train it using solely along-track measures and compare it with its classically su-
117 pervised version.

118 This paper is structured as follows, in Section 2 after giving a rationale for the inclu-
119 sion of SST information in the interpolation method we detail our OSSE. In Section 3
120 we present our architecture and the training losses. In Section 4 we evaluate the inter-

121 polation in terms of SSH reconstruction, and oceanic circulation errors. We also perform
 122 an eddy detection to demonstrate that SST-using methods retrieve more realistic ocean
 123 structures and we compare ourselves to existing state-of-the-art methods on a different
 124 OSSE. In Section 5, we discuss the limitations and perspectives of this work.

125 2 Multi-variate data simulation

126 In the following, we provide a rationale for the SSH and SST connection, outline
 127 the reference data source we utilized (Global Ocean physics Reanalysis (CMEMS, 2020)),
 128 and detail our OSSE’s SSH and SST observations.

129 2.1 Physical relationship between SSH and SST

130 One of the most important uses of SSH data is to recover oceanic currents through
 131 surface quasi-geostrophic approximation. It consists of supposing a static equilibrium
 132 between the surface projection of the Coriolis force and the resultant pressure forces. Far
 133 from the Equator, where Coriolis force projection is null, it is a good estimation of the
 134 circulation. The surface geostrophic currents can be computed from the SSH h follow-
 135 ing:

$$\mathbf{w}_{geo} = \begin{pmatrix} u_{geo} \\ v_{geo} \end{pmatrix} = \begin{pmatrix} -\frac{g}{f} \frac{\partial h}{\partial y} \\ \frac{g}{f} \frac{\partial h}{\partial x} \end{pmatrix} \quad (1)$$

136 where u_{geo} and v_{geo} are the eastward and northward geostrophic currents, x and y the
 137 eastward and northward coordinates and where $f = 2\Omega_r \sin(\phi)$ is the Coriolis factor,
 138 Ω_r being the rotation period of the earth, ϕ the latitude and g the gravitational accel-
 139 eration.

140 In a first approximation, the surface temperature T can be considered as a passive
 141 tracker transported by surface currents. The evolution of a scalar in a static velocity field
 142 can be described by the linear advection equation.

$$\frac{\partial T}{\partial t} + \mathbf{w} \cdot \nabla T = 0 \quad (2)$$

143 Combining the geostrophic and the advection Equations (1,2), we see why a time series
 144 of SST observations should provide pertinent information for constraining the SSH re-
 145 construction. However, the actual physical link between temperature and sea-surface height
 146 is more complex, as other phenomena must be considered, such as diffusion, convection,
 147 circulation between water depths, and viscosity. The satellite observations of both tem-
 148 perature and sea surface height also suffer from instrumental errors and are by nature
 149 limited to observing the surface of the ocean. This is why neural network architectures,
 150 thanks to their flexibility, seem appropriate to learn the complex underlying link between
 151 the data.

152 2.2 Observing System Simulation Experiment

153 In order to effectively replicate the relationship between the two variables, we pro-
 154 pose an Observing System Simulation Experiment (OSSE), meaning a twin experiment
 155 that accurately models the satellite observations of the Ocean. This approach is widely
 156 used in the geosciences community as it provides ways to test reconstruction methods
 157 and errors (Amores et al., 2018; Stegner et al., 2021; Gaultier et al., 2016). With this
 158 mindset, SSH and SST variables of a high-resolution simulation are considered as the
 159 ground truth ocean state upon which we simulate satellite measures. The coherence of

160 the relation between SSH and SST is ensured by the physical model, while with our OSSE
 161 we produce enough pairs of ground truth/observation to train a neural network. In this
 162 paper, we denote \mathbf{X}^{ssh} and \mathbf{X}^{sst} the ground truth fields of the SSH and SST and \mathbf{Y}^{ssh}
 163 and \mathbf{Y}^{sst} , the simulated observations. We detail hereafter the reference dataset of our
 164 OSSE and the observation operators of the two variables.

165 **2.2.1 Base simulation**

166 We conduct our experiences on the Global Ocean physics Reanalysis product (GLO-
 167 RYS12) (CMEMS, 2020). It provides various physical data such as SSH, SST and oceanic
 168 currents with a spatial resolution of $1/12^\circ$ (around 8 km). GLORYS12 is based on the
 169 NEMO 3.6 model (Madec et al., 2017) and assimilates observations from satellites (SSH
 170 along-track observations and SST full domain observations) through a reduced-order Kalman
 171 filter. It is updated annually by the Copernicus European Marine Service, making it im-
 172 possible to use in near real-time applications. We select a temporal subset of this sim-
 173 ulation from Mars 20, 2000 to December 29, 2019, for a total of 7194 days.

174 We select a portion of the Golf stream, between 33° to 43° North and -65° to -55°
 175 East. This area is known for its intense circulation, its water mass of very different tem-
 176 peratures, and is far enough from the equator that the geostrophic approximation can
 177 be applied. Comparing the surface circulation of the model with its geostrophic approx-
 178 imation, we find that an RMSE of 6.6 cm/s for u_{geo} and 6.1 cm/s for v_{geo} . Consider-
 179 ing the high intensity and variations of the currents in the Golf stream (with 37.1 and
 180 34.3 cm/s of standard deviation for u and v respectively), geostrophy seems to be an ad-
 181 equate estimation. Thus, we expect a significant synergy between SSH and SST which
 182 can be learned by a neural network. For computational reasons, we resample the data
 183 to images of size 128×128 with a bilinear interpolation, corresponding to a resolution
 184 of 0.078° by pixel (approximately 8.7 km). Doing so, the receptive field of the network
 185 covers the entire 10° by 10° area.

186 **2.2.2 SSH observations**

187 The nadir-pointing altimetry satellites take approximately a measurement per sec-
 188 ond, along their ground tracks. Their observations are a series of values with precise spa-
 189 tiotemporal coordinates that we aim to simulate. To do so, we retrieve the support of
 190 real-world satellite observations denoted $\mathbf{\Omega} = \{\Omega_i = (t_i, lat_i, lon_i), i \in [0 : N]\}$ from the
 191 Copernicus sea level product (CMEMS, 2021). Using $\mathbf{\Omega}$ and the ground truth data \mathbf{X}^{ssh}
 192 we simulate SSH observations \mathbf{Y}^{ssh} as the trilinear interpolation of the simulated field
 193 on each point of the support. We add an instrumental error $\varepsilon \sim \mathcal{N}(0, \sigma)$ with $\sigma = 1.9 \text{ cm}$,
 194 which is the distribution used in the Ocean data challenge 2020 (CLS/MEOM, 2020).
 195 The SSH observations \mathbf{Y}^{ssh} is defined as following:

$$\mathbf{Y}^{ssh} = \mathcal{H}^{ssh}(\mathbf{X}^{ssh}, \mathbf{\Omega}) + \varepsilon \quad (3)$$

196 where \mathcal{H}^{ssh} is the trilinear interpolation operator of the ground truth \mathbf{X}^{ssh} on the sup-
 197 port $\mathbf{\Omega}$. An example of these simulated along-track measurements is presented on the
 198 first row of Figure 1. For the neural network input observations, we regrid these data
 199 to a daily 128×128 image. We set the pixel value with no simulated satellite observa-
 200 tion to zero and we average the daily measures of SSH inside each pixel so that it rep-
 201 represents the mean of the daily measures from the different satellites (if any). As the GLO-
 202 RYS12 simulation assimilates SSH alongracks measurements, we introduce a delay be-
 203 tween the L3 satellite observations and the simulation. Doing so, we ensure that sim-
 204 ulated along-tracks are taken randomly and not specifically where the model assimilated
 205 real world observations.

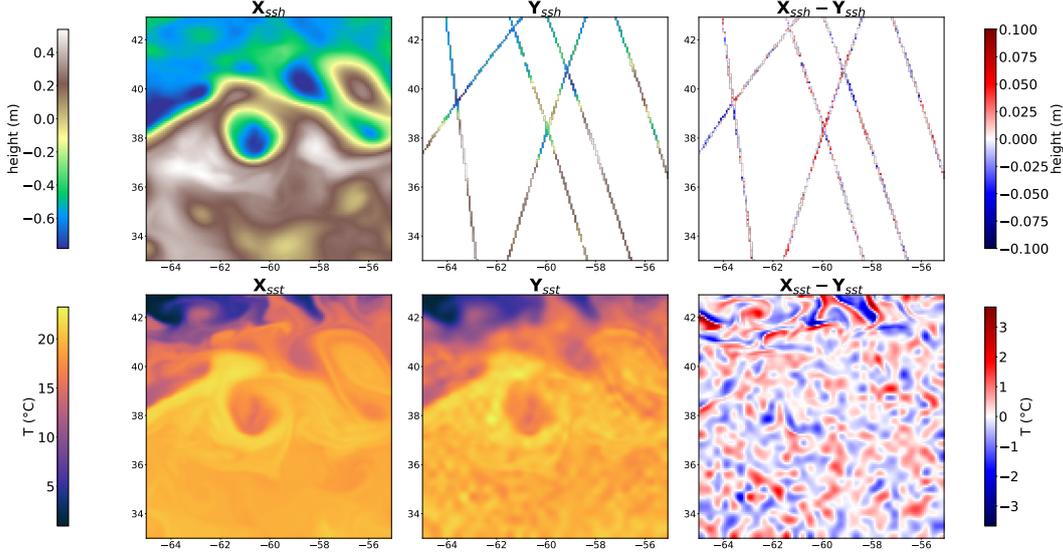


Figure 1. Images of the Ground Truth variables from GLORYS and the simulated satellite observations. The first row is the SSH variable, where the second row is the SST. The first column is the ground truth from GLORYS simulation, the second column is their associated satellite observation and the last is the difference.

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2.2.3 SST observations

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SST remote sensing is based on direct infrared measurements, leading to wider measurement swaths but making the measurement sensible to cloud cover. The so-called L3 satellite products have much higher data coverage, but no observation is possible when the cloud is too thick. To fill the gaps, the L3 products from several satellites are merged and interpolated to form the fully gridded image. This results in various resolutions in the same product, where high-resolution structures are artificially smoothed when the cloud coverage is too thick. To simulate this process, we use the mask of NRT L3 product (CMEMS, 2023) to retrieve a realistic cloud cover mask C (between 0 and 1) which we grid to the target resolution. The SST observation operator \mathcal{H}^{sst} can then be written as:

$$\mathbf{Y}^{sst} = \mathcal{H}^{sst}(\mathbf{X}^{sst}, C) = (1 - C) \odot (\mathbf{X}^{sst} + \varepsilon) + C \odot \mathcal{G}_{\sigma} \star (\mathbf{X}^{sst} + \varepsilon) \quad (4)$$

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where \odot is the element-wise product, \star the convolution product, ε is a white Gaussian noise image of size 32×32 linearly upsampled to a 128×128 image. We also use a spatial Gaussian filter (\mathcal{G}_{σ}) with $\sigma = 16(\text{km})$ to simulate the smoothing of the interpolation performed by satellite products. Our SST observations thus present a spatially and temporally correlated noise, with different resolutions depending on cloud coverage. In the end, \mathcal{H}^{sst} adds a noise with a standard deviation of 0.5°C where the SST standard deviation of the ground truth is 4.96°C . This observation operator is different from real-world degradations but produces an image with an in-equal noise resolution similar to the errors present in the L4 SST products.

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3 Proposed interpolation method

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3.1 Learning the interpolation

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The observation operator \mathcal{H}^{ssh} previously described can be seen as a forward operator that we aim to inverse. In the past years, deep neural networks, and especially convolutional neural networks, have proven their ability to solve ill-posed image inverse

231 problems (McCann et al., 2017) and more specifically inpainting problems (Jam et al.,
 232 2021; Qin et al., 2021). A neural network f_θ is trained on a database to estimate the true
 233 state from observations $f_\theta(y) = \hat{x}$. Learning this inversion operator thus requires (y, x)
 234 pairs (supervised) or only y (unsupervised) (Ongie et al., 2020).

235 We chose to perform the interpolation on a time window of 21 days, the input is
 236 thus a tensor of 21 images of SSH, with or without SST images, and the output is the
 237 21 corresponding days of SSH only. An overview of the inputs and outputs of our method
 238 is provided in Figure 3. The neural network estimates the true state from observations,
 239 $\hat{\mathbf{X}}^{ssh} = f_\theta(\mathbf{Y})$, where $\mathbf{Y} = \mathbf{Y}^{ssh}$ for a SSH-only interpolation, and $\mathbf{Y} = (\mathbf{Y}^{ssh}, \mathbf{Y}^{sst})$
 240 if the network uses SST. The length of the time window will be discussed in Section 4.1,
 241 and training losses of the network in Section 3.3.

242 3.2 Architecture

243 We propose an attention-based encoder-decoder (ABED) presented in Figure 2 to
 244 perform the interpolation over the time window. The attention mechanism allows to em-
 245 phasize important features while neglecting irrelevant ones which makes it well-suited
 246 to extract information from contextual variables. It is widely used in many computer
 247 vision tasks (Guo et al., 2021) and can be transposed to geoscience applications. The
 248 overall structure of our neural network is inspired by the one used by Che et al. (2022)
 249 that introduced a residual Unet with attention layers for rain nowcasting.

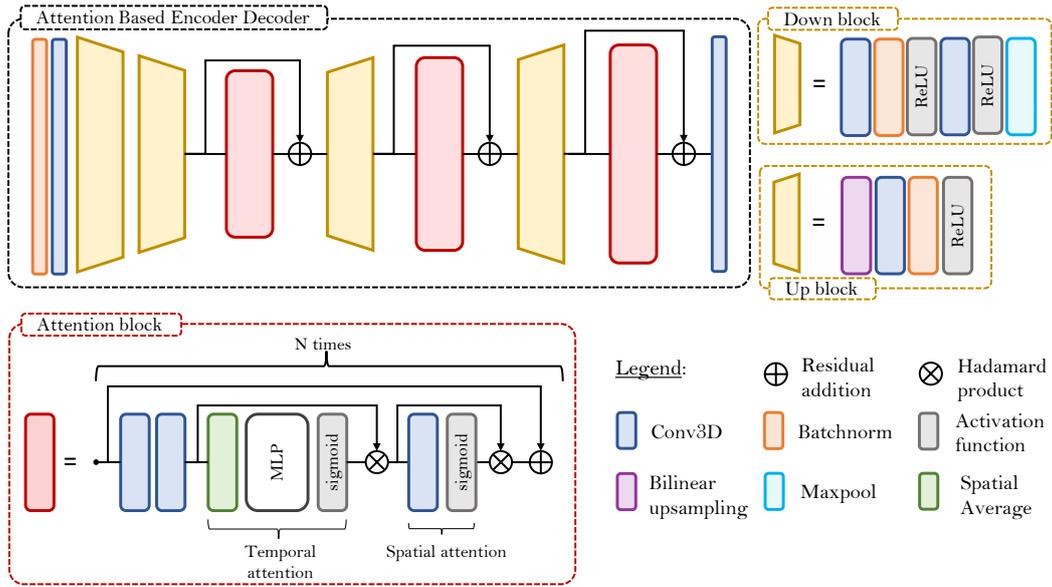


Figure 2. The architecture of the proposed Attention-Based Encoder Decoder (ABED) neural network. It is designed to take a time series of 21 images of SSH, with or without a time series of SST. The encoder divides the spatial dimensions of the images by 4 through 2 “down-block”. Then the decoder uses an attention block to highlight relevant information in the images and progressively upscales it.

250 The encoder starts with a batch normalization and a 3D convolution (in time and
 251 in the two spatial dimensions) followed by two downsampling blocks that divide spatial
 252 dimensions by 2 (see Figure 2). The decoder is composed of residual attention blocks fol-
 253 lowed by upsampling blocks.

254 We describe hereafter our attention block which consists of two essential steps: tempo-
 255 ral attention and spatial attention. Our approach builds upon the Convolutional Block
 256 Attention Module (CBAM) principle introduced by Woo et al. (2018), which successively
 257 performs channel and spatial attention. We extend this idea by incorporating tempo-
 258 ral information in the channel attention mechanism. To do so, we first compute the spa-
 259 tial average of each channel and instant, resulting in a tensor of size $C \times T$ where C
 260 is the channel number and T is the time series length. Subsequently, we apply two one-
 261 dimensional convolutional layers with a kernel of size 1, followed by a sigmoid activation
 262 function to estimate the attention weights. This corresponds to a 2-layer perceptron shared
 263 by every time step, which is different from the CBAM, as it includes the temporal in-
 264 formation in the channel attention. These weights are then multiplied to each timestep
 265 of every channel, enabling the network to highlight salient features and suppress irrel-
 266 evant information. After performing temporal attention, we proceed with spatial atten-
 267 tion. This step involves utilizing a 3-dimensional convolutional operation, where the tem-
 268 poral length of the kernel size matches the length of the time series. As a result, the en-
 269 tire time series is aggregated into a single 2D image, which serves as the basis for deriv-
 270 ing spatial attention. A residual skip connection is then applied, and the described block
 271 is repeated 4, 2, and 1 time for the first, second, and last block respectively. For further
 272 details about our implementation, we provide the PyTorch implementation of our net-
 273 work in https://gitlab.lip6.fr/archambault/james_2023.

274 3.3 Loss and regularization

275 We propose to compare two main strategies to train the neural network. Thanks
 276 to the OSSE previously described, we have access to the ground truth which we can use
 277 to learn the interpolation in a classic supervised fashion. However, it is also possible to
 278 train directly on observations, by applying the observation operator \mathcal{H}^{ssh} on the gen-
 279 erated map $\hat{\mathbf{X}}^{ssh}$ before computing the loss (see Equations 5,6,7). Filoche et al. (2022)
 280 performed the interpolation with SSH observations only, and, using the same principle,
 281 Archambault et al. (2023) showed that it was possible to overfit SSH images starting from
 282 SST only and constraining on SSH observations. Both these methods are fitted on one
 283 (or a small number) of examples and must therefore be refitted in order to be applied
 284 to unseen data. Using a larger real-world satellite dataset, S. A. Martin et al. (2023) trained
 285 a neural network directly from observations, by constraining it on independent satellite
 286 observations that were not given in the input. However, the lack of ground truth refer-
 287 ence makes it harder to compare the different reconstructions, especially regarding de-
 288 tected eddies and structures. We propose to train neural networks using the 3 follow-
 289 ing losses:

- 290 • The MSE using ground truth :

$$\mathcal{L}(\mathbf{X}^{ssh}, \hat{\mathbf{X}}^{ssh}) = \frac{1}{T \times H \times W} \sum_{t,x,y} (\mathbf{X}_{t,x,y}^{ssh} - \hat{\mathbf{X}}_{t,x,y}^{ssh})^2 \quad (5)$$

- 291 • The MSE using only observations:

$$\mathcal{L}_{trili}(\mathbf{Y}^{ssh}, \hat{\mathbf{X}}^{ssh}) = \frac{1}{N} \sum_i (\mathbf{Y}_i^{ssh} - \mathcal{H}^{ssh}(\hat{\mathbf{X}}^{ssh})_i)^2 \quad (6)$$

- 292 • The MSE using only observations and the regularization introduced by S. A. Mar-
 293 tin et al. (2023):

$$\begin{aligned} \mathcal{L}_{trili_reg}(\mathbf{Y}^{ssh}, \hat{\mathbf{X}}^{ssh}) = & \mathcal{L}_{trili}(\mathbf{Y}^{ssh}, \hat{\mathbf{X}}^{ssh}) + \lambda_1 \frac{1}{N_1} \sum_i \left(\frac{\partial}{\partial s} \mathbf{Y}_i^{ssh} - \frac{\partial}{\partial s} \mathcal{H}^{ssh}(\hat{\mathbf{X}}^{ssh})_i \right)^2 \\ & + \lambda_2 \frac{1}{N_2} \sum_i \left(\frac{\partial^2}{\partial s^2} \mathbf{Y}_i^{ssh} - \frac{\partial^2}{\partial s^2} \mathcal{H}^{ssh}(\hat{\mathbf{X}}^{ssh})_i \right)^2 \end{aligned} \quad (7)$$

294 where $\frac{\partial}{\partial s}$ is the along-track derivation of the SSH approximated by its rate of change (see
 295 Appendix 6.1). T is the temporal length of the time series (here 21), H and W the spa-
 296 tial dimensions of the images (here both equals 128), and N , N_1 , N_2 , the number of satel-
 297 lite measures of SSH, and SSH first and second along-track spatial derivative respectively.
 298 We take $\lambda_1 = \lambda_2 = 0.05$ the regularization coefficients, the same values used by S. A. Mar-
 299 tin et al. (2023).

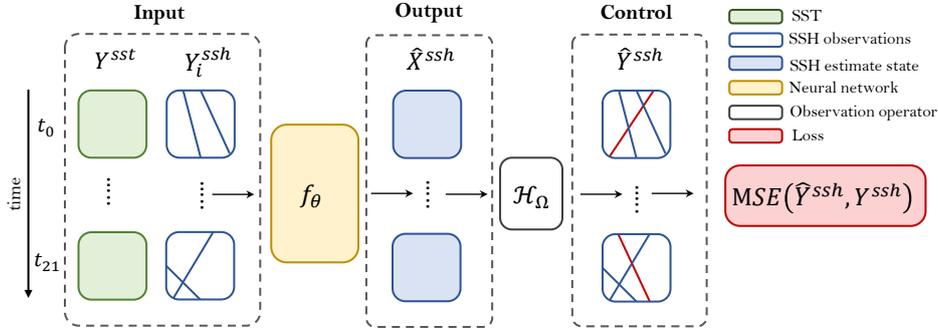


Figure 3. Computational graph of the proposed unsupervised interpolation method. The input of the neural network is a 21-day time series of SSH satellite observations, excluding data from a single satellite, and optionally includes SST measurements. The network estimates a time series of SSH fields states, upon which the observation operator is subsequently applied in order to deduce \hat{Y}^{ssh} . Finally the Mean Squared Error between the \hat{Y}^{ssh} and Y^{ssh} is used to control the network.

300 The losses \mathcal{L}_{trili} and $\mathcal{L}_{trili.reg}$ apply the observation operator \mathcal{H}^{ssh} , before
 301 computing the MSE, which allows the training in a framework where only observations are
 302 available. Thus, from an interpolation point of view, the inversion methods that use these
 303 losses are unsupervised as they can be trained without any ground truth image. How-
 304 ever, if we constrain the network on the same observations that were given in input, an
 305 over-fitting of along tracks will occur with no guarantee of generalization. To avoid this
 306 problem, we remove the measure from one satellite from the input of the network but
 307 calculate the loss function on all satellite observations. Doing so, the network must gen-
 308 eralize outside the along-track measure that was given as input. In Figure 3 we call Y_i^{ssh}
 309 the input observations and present an unsupervised inversion computational graph.

310 3.4 Training details

311 **Train, validation, test split.** We partitioned the dataset into three subsets: training,
 312 validation, and test data. We used the year 2017 exclusively for testing our reconstruc-
 313 tions (every analysis conducted in the following was performed on this data). We val-
 314 idate our methods on three distinct time intervals: (1) from July 14, 2002, to July 28,
 315 2003, (2) from January 5, 2008, to January 18, 2009, and (3) from June 28, 2013, to July
 316 13, 2014. The remaining data was used for training, with the exception of a 15-day pe-
 317 riod set aside to prevent data leakage.

318 **Normalization.** We normalize both the input and output of the artificial network. This
 319 involves subtracting the mean and dividing by the standard deviation, which are both
 320 computed on the entire training dataset. Specifically, for images related to SSH measure-
 321 ments along tracks, we first perform this normalization and subsequently replace any miss-
 322 ing values with zeros. We normalize the neural network SSH outputs with the statistics
 323 computed on the input observations (in order that the method remains applicable in an
 324 unsupervised setting).

325 **Training hyperparameters.** We train every method using an ADAM optimizer (Kingma
 326 & Ba, 2017) with a learning rate starting at 5.10^{-5} and a decay of 0.99. We perform an
 327 early stopping with a patience of 8 epochs. For the supervised training the stopping cri-
 328 teria is the RMSE of the reconstruction on the fully gridded domain on the validation
 329 data, but in the unsupervised setting, we compute this RMSE on left-aside along-track
 330 measures. Doing so, the stopping strategy is still compliant with a situation where no
 331 ground truth is accessible.

332 **Ensemble.** As neural network optimization is sensible to its weight initialization, we
 333 train 3 networks for every setting. The so-called “Ensemble” estimation is the average
 334 SSH map of the 3 networks. Performing an ensemble estimation helps to stabilize per-
 335 formances, and even enhance the reconstruction (Hinton & Dean, 2015). In the follow-
 336 ing, we call “Ensemble score” the score of the previously mentioned ensemble estima-
 337 tion, and “Mean score” the average of the score of each network taken independently.

338 4 Results

339 In the following, we present the scores of the different reconstruction methods on
 340 the test set. In contrast to the training and validation method, we assess the quality of
 341 the reconstruction on the gridded ground truth. We compare the fields estimated by the
 342 3 losses \mathcal{L} , \mathcal{L}_{tri} and $\mathcal{L}_{tri.reg}$ on 3 different sets of input data: one with only SSH tracks,
 343 one with SSH and the noised SST denoted nSST, and one with the noise-free SST of the
 344 GLORYS assimilation. We train interpolation methods on noise-free SST to provide an
 345 upper-bound performance of the neural network in the case of a perfect physical link be-
 346 tween SSH and SST.

347 4.1 SSH reconstruction and quality of derived geostrophic currents

348 We give the RMSE of the SSH estimates fields in Table 1, and the RMSE on the
 349 velocity fields in Table 2. As expected, the supervised loss function outperforms the un-
 350 supervised framework in every data scenario. Specifically, in the SSH+SST scenario, the
 351 supervised loss decreases the RMSE of \mathcal{L}_{tri} by 24%, and 8% without SST. Also, adding
 352 SST as an additional input to the network generally leads to improved performance com-
 353 pared to using SSH alone. This improvement is observed across all three loss functions,
 354 as the error values decrease for SSH+nSST compared to SSH. For instance, the SSH-
 355 only RMSE is decreased by 30% and 23% for SST and nSST respectively with \mathcal{L} . The
 356 regularization introduced by (S. A. Martin et al., 2023) slightly increases reconstruction
 357 but is still close to the unregularized inversion.

358 We estimate the surface currents from the reconstructed SSH from Equation 1, and
 359 we compare it to the surface circulation of the model. The errors on velocity in Table 2
 360 follow the same patterns as the RMSE on the SSH fields but with lesser differences be-
 361 tween methods. The RMSE is not too far from the minimal error achievable through geostro-
 362 phy, which is 6.57 cm/s for u and 6.14 for v on this data.

363 In Figure 4, we show the daily errors of the different methods on the test year. We
 364 notice a strong temporal variability of the RMSE with a notable increase over late Sum-
 365 mer. Specifically, in August and September, all methods are performing worse than in
 366 Winter which can be explained by the high energy of the Ocean at this period.

367 An important challenge of ocean satellite products is providing real-time estima-
 368 tions, as many applications cannot use products available with too much time delay. In
 369 an operational framework, products that are immediately available are called Near Real
 370 Time (NRT) whereas those that require a time delay before release are called Delayed
 371 Time (DT). While in Table 1 we presented the results obtained on the central image of
 372 the time window, we can also display their scores along the 21-days temporal window

Loss	SSH	SSH+nSST	SSH+SST
\mathcal{L} (supervised)	4.18 — 3.85	3.23 — 2.93	2.92 — 2.59
\mathcal{L}_{tri}	4.52 — 4.16	3.86 — 3.51	3.62 — 3.24
\mathcal{L}_{tri_reg}	4.38 — 4.13	3.73 — 3.48	3.48 — 3.20

Table 1. SSH reconstruction RMSE in centimeters (mean score on the left and ensemble score on the right) of 3 ABED networks. The interpolation is trained using the 3 different losses described in Section 3.3 with the following settings: SSH-only interpolation, SSH and noised SST, and SSH and noise-free SST. All metrics are given on the central image of a 21-day time window.

Loss	SSH		SSH+nSST		SSH+SST	
	<i>u</i>	<i>v</i>	<i>u</i>	<i>v</i>	<i>u</i>	<i>v</i>
\mathcal{L}^*	13.0	14.1	10.9	11.7	10.1	10.6
\mathcal{L}_{tri}	13.3	15.7	12.1	14.2	11.3	13.4
\mathcal{L}_{tri_reg}	12.9	14.3	11.8	12.9	11.1	12.1

*supervised

Table 2. Eastward (*u*) and northward (*v*) surface currents in cm/s. The currents were estimated by applying the geostrophy approximation (see Equation 1) on the SSH ensemble estimation of the 3 ABED networks.

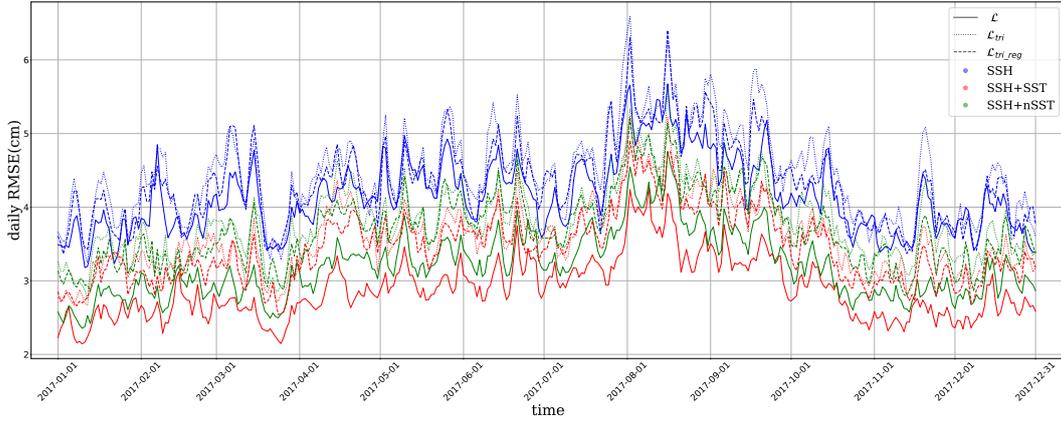


Figure 4. RMSE of the different reconstructions during the test year (2017)

373 as in Figure 5. The central image is a 10-day Delayed Time reconstruction as we need
 374 images of observations 10 days in the future. In Figure 5 we can verify that 21 days of
 375 data contain enough information to reconstruct the central image: for instance, 5 days
 376 from the border of the temporal window the reconstruction error is just 3% higher than
 377 the one at the center. This means that we can significantly reduce the delay (and there-
 378 fore the training cost of our model) without causing severe drops in performance, which
 379 could be useful if applied in an operational framework. However, when it comes to pro-
 380 ducing NRT products (0 delay) this graph shows that we expect a significant loss of qual-
 381 ity in the reconstruction which is usual (Amores et al., 2018; Stegner et al., 2021). To
 382 accurately produce an NRT image and even forecast, different training methods should

383

be tested such as centering the target time window in the future compared to observations.

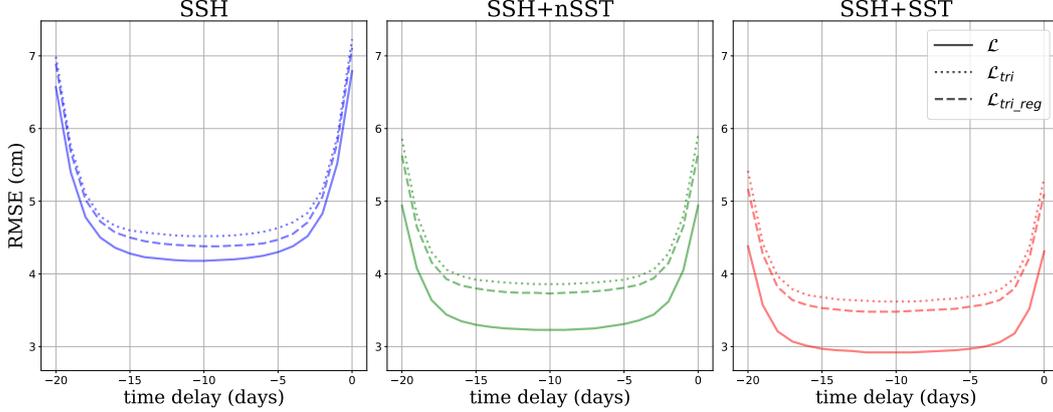


Figure 5. RMSE of the different reconstructions along the time window. The errors at a time delay of -20 correspond to an anti-causal scheme (knowing only future observations) whereas $timedelay = 0$ corresponds to a causal scheme (knowing no future observations). Knowing both past and future observations leads to the optimal reconstruction at $timedelay = -10$.

384

4.2 Eddy detection analysis

385

4.2.1 Importance of mesoscale eddies

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Mesoscale eddies play an important role in ocean circulation and dynamics and their understanding leads to diverse applications in oceanography or navigation (Chelton, Schlax, & Samelson, 2011). Previous studies underline how these structures transport heat, especially between latitudes 0° and 40° in the North Atlantic (Jayne & Marotzke, 2002), but also salinity (Amores et al., 2017), or plankton (Chelton, Gaube, et al., 2011). In practice, mesoscale eddies and structures are estimated through geostrophic currents derived from satellite altimetry. However, operational satellite products such as DUACS, have too coarse resolutions to resolve accurately mesoscale structures. Performing an OSSE to simulate the satellite’s remote sensing Amores et al. (2018); Stegner et al. (2021) showed that DUACS-like optimal interpolation aggregates small eddies into larger ones (i.e. with a radius greater than 100 km). These interpolations also capture a small percentage of eddies present in the model simulation (around 6% in the North Atlantic) and change the eddies’ distribution and properties. This is why we are interested in finding to what extent our reconstruction methods are able to detect small eddies in the ground truth, and how well the detected eddies are resolved and their physical properties conserved.

401

402

4.2.2 Automatic eddy detection algorithm: AMEDA

403

We use the Angular Momentum for Eddy Detection and tracking Algorithm (AMEDA) introduced by (Vu et al., 2018) to perform the eddies detection. It is based on the Local Normalized Angular Momentum (LNAM), a dynamic metric first introduced by (Mkhinini et al., 2014), that we define hereafter:

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405

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$$LNAM(P_i) = \frac{\sum_j \overrightarrow{P_i P_j} \times \overrightarrow{V_j}}{\sum_j \overrightarrow{P_i P_j} \cdot \overrightarrow{V_j} + \sum_j |\overrightarrow{P_i P_j}| |\overrightarrow{V_j}|} = \frac{L_i}{S_i + BL_i} \quad (8)$$

407 where P_i is the point of the grid where we compute the LNAM, P_j is a neighbor point
 408 of the grid, $\overrightarrow{P_i P_j}$ is the position vector from P_i to P_j and $\overrightarrow{V_j}$ is the velocity vector in P_j .
 409 Thus, the unnormalized angular momentum L_i is computed through a sum of cross prod-
 410 ucts and is bounded by BL_i , so that if P_i is the center of an axisymmetric cyclone (resp
 411 anticyclone), $LNAM(P_i)$ will be equal to 1 (resp -1). Also, if the circulation field is hy-
 412 perbolic and not an ellipsoid, S_i will reach large values, and $LNAM(P_i)$ will be close
 413 to 0. All sum is computed on a local neighborhood of P_i , which is a hyperparameter of
 414 the method (typically a square centered in P_i).

415 AMEDA finds potential eddy centers by searching for the local extrema of the $LNAM$
 416 field. The shapes of the eddies are then defined by following closed current streamlines
 417 (either taking the last closed streamline, or the maximum velocity one). We perform the
 418 AMEDA algorithm on the geostrophic velocity field of our estimation and on the ground
 419 truth currents. An eddy is said to be detected if its ground truth barycenter is inside
 420 the closed streamline of its estimation.

421 4.2.3 Eddy detection performances

422 We present hereafter the detection scores of the different reconstruction methods,
 423 with three data scenarios and three losses. We take the ensemble SSH estimation of the
 424 neural networks and perform the AMEDA algorithm on the velocity field derived through
 425 the geostrophic approximation (see Equation 1).

426 In Table 3 we present the F_1 score, the recall, and the precision of the methods.
 427 The recall tells us the proportion of actual positive instances that were correctly iden-
 428 tified by the detection (a recall of 1 means that all ground truth eddies were detected).
 429 The precision measures the trust that we can put in the detected eddies (a precision of
 430 1 means that all eddies in the simulation were also present in the ground truth). To ag-
 431 gregate the recall and the precision, we use the F_1 score which is the harmonic mean of
 432 recall and precision. A value of 1 means a perfect detection: all ground truth eddies were
 433 detected and the estimation produced no false positive.

Loss	SSH			SSH+nSST			SSH+SST		
	F_1	recall	precision	F_1	recall	precision	F_1	recall	precision
\mathcal{L} (supervised)	0.719	0.617	0.86	0.765	0.685	0.866	0.785	0.728	0.852
\mathcal{L}_{tri}	0.704	0.647	0.771	0.727	0.672	0.79	0.739	0.692	0.793
\mathcal{L}_{tri_reg}	0.714	0.609	0.863	0.725	0.623	0.865	0.742	0.644	0.877

Table 3. Scores of the AMEDA eddy detection performed on the Ensemble estimation of ABED interpolation. The considered scores are the precision, the recall, and the F_1 score.

434 **Data comparison.** As expected, no matter which loss we consider, the detection method
 435 using noise-free temperature outperforms the two other scenarios with higher F_1 scores.
 436 Even the noisy SST provides important information for eddy reconstruction as the SSH-
 437 only method yields lower results than the two other scenarios. We also see that for each
 438 loss, the precision scores are less impacted by the input data than the recall is. This means
 439 that the SSH-only scenario does not produce a lot more false detection than the SST meth-
 440 ods, but misses much more structures.

441 **Loss comparison.** On the other hand, the loss function used to perform the inversion
 442 has a substantial impact on precision and recall. The regularization of the unsupervised
 443 loss brings the detection precision to the level of the supervised method (even higher for
 444 the SSH-only and SSH+SST) but also reduces the recall of all methods compared to their

445 unregularized version. In other words, adding a smoothness constraint on the SSH gra-
 446 dient field prevents the neural network from generating false eddies, but also prevents
 447 it from retrieving some structures.

448 **4.2.4 Physical properties of detected eddies**

449 In order to further investigate the performance of the eddy detection methods, we
 450 analyze the detection outcomes based on the physical characteristics of the eddies. For
 451 instance, smaller eddies tend to have shorter lifespans, making them more challenging
 452 to detect due to their decreased likelihood of being observed by satellites. Conversely,
 453 high-speed eddies are derived from important sea surface height (SSH) variations, thus
 454 exhibiting a strong signature in the generated mapping. Figure 6 shows the detection
 455 performances as a function of some key parameters such as the maximum radius, life-
 456 time, or maximum velocity along the final closed current line.

457 As anticipated, using SST and nSST data contributes to the detection of eddies,
 458 as indicated by the higher F_1 scores achieved in every loss scenario. However, small and
 459 short-lived eddies are less frequently detected, resulting in lower recall scores. Specifi-
 460 cally, only 17% of the eddies with a radius below 15 km are successfully detected in the
 461 best scenario. Nonetheless, except for the unregularized trilinear loss function, the pre-
 462 cision scores for the detected eddies remain high, even for small and short-lived ones. This
 463 observation confirms the previously observed phenomenon where the regularization em-
 464 ployed in the inversion process prevents the network from generating false eddy detec-
 465 tions, but also stops it from capturing a significant portion of the actual eddies. This reg-
 466 ularization behavior is expected, as forcing a smoothness constraint on the SSH gradi-
 467 ent field leads to denying some of the small structures.

468 We also want to assess the accuracy of the model to estimate the physical prop-
 469 erties of the eddies. To this end, we focus on the eddies that were successfully detected
 470 by all the methods (4881 eddies out of the 7908 eddies in the ground truth). We com-
 471 pare the physical parameters of the estimated eddies to their values in the correspond-
 472 ing true eddy. To do so, we compute the RMSE and bias of the following parameters:
 473 the maximum radius and velocity, and the average distance between the centers of es-
 474 timate and true eddies. The error RMSE tells us if the eddies are well resolved, whereas
 475 the bias (estimate parameter minus ground truth parameter) tells us if the interpolation
 476 method has a global tendency to overestimate or underestimate some characteristics of
 477 the eddies.

478 Once again, Tables 4, 5 and 6 show that SST helps to estimate eddies radius, ve-
 479 locity, and position. Nonetheless, there is a bias of radius and velocity: the size of the
 480 eddy is statistically overestimated compared to its ground truth, while its speed is sys-
 481 tematically underestimated. This is particularly true for the regularized unsupervised
 482 loss because of its smoothness constraint, with a velocity bias accountable for half of the
 483 RMSE. It could be interesting to know if the estimated eddies could be unbiased with-
 484 out decreasing the other performances.

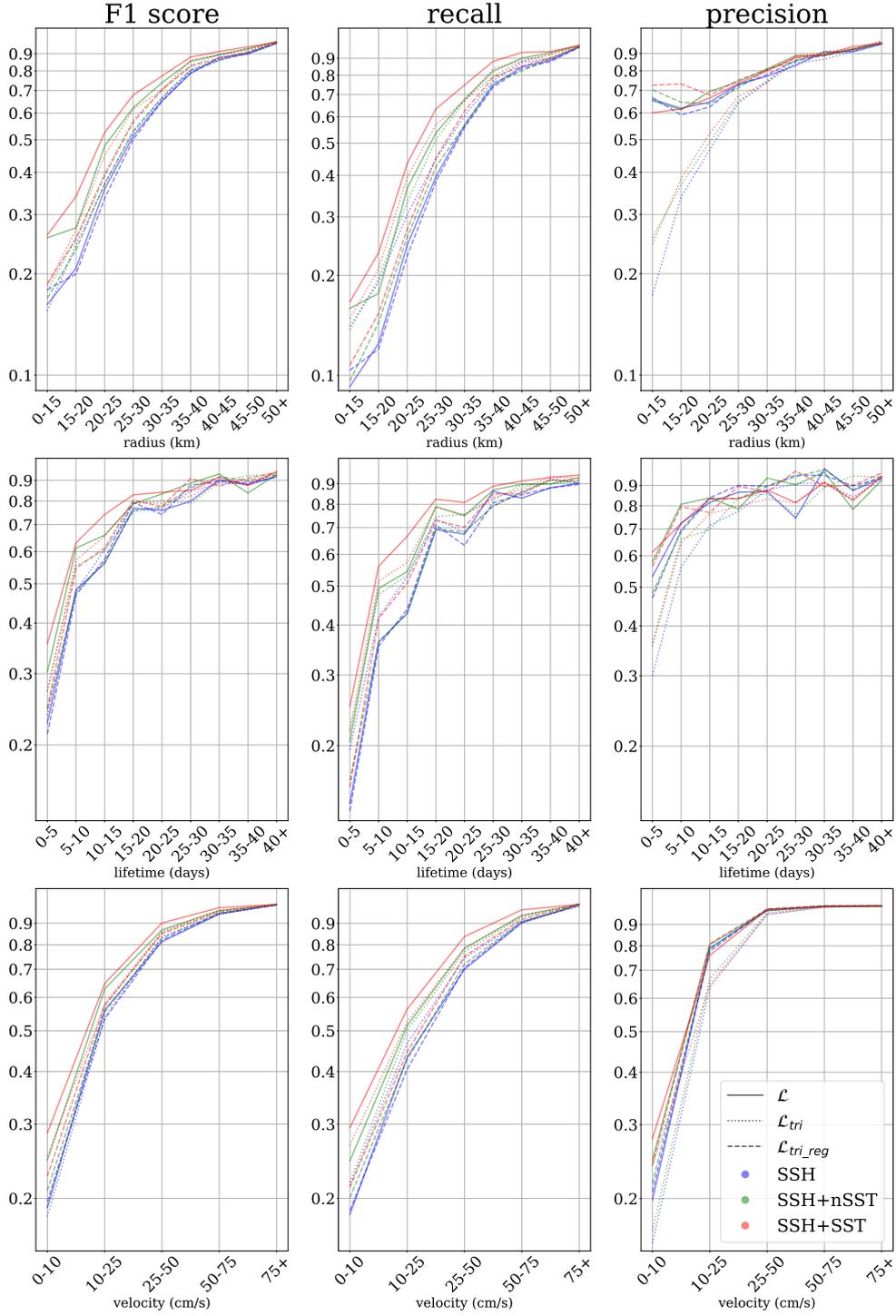


Figure 6. Detection scores of the different methods on eddies separated by radius (first row), lifetime (second row), and maximum velocity (last row). The considered scores are F_1 (first column), recall (second column), and precision (third column). The recall tells the proportion of actual positive instances that were correctly identified, the precision measures the trust that we can put in the detected eddies, and the F_1 score aggregates these two values.

Loss	SSH		SSH+nSST		SSH+SST	
	RMSE	bias	RMSE	bias	RMSE	bias
\mathcal{L} (supervised)	21.8	3.8	20.5	4.5	19.0	3.8
\mathcal{L}_{tri}	21.5	1.6	20.4	2.2	20.8	1.7
$\mathcal{L}_{tri.reg}$	22.4	2.9	21.7	3.3	21.2	3.9

Table 4. Eddies maximum radius RMSE and bias (km). The eddy detection is performed on geostrophic currents of the ensemble estimation and the bias is computed from the estimated radius minus ground truth radius

Loss	SSH		SSH+nSST		SSH+SST	
	RMSE	bias	RMSE	bias	RMSE	bias
\mathcal{L} (supervised)	12.9	-6.2	11.0	-3.8	10.2	-2.4
\mathcal{L}_{tri}	12.7	-5.3	11.9	-4.5	12.2	-3.8
$\mathcal{L}_{tri.reg}$	13.8	-8.0	13.0	-6.9	12.1	-5.8

Table 5. Eddies maximum velocity RMSE and bias (cm/s)

Loss	SSH	SSH+nSST	SSH+SST
	RMSE	RMSE	RMSE
\mathcal{L} (supervised)	23.2	21.7	20.3
\mathcal{L}_{tri}	24.5	23.5	22.9
$\mathcal{L}_{tri.reg}$	23.4	23.2	22.2

Table 6. Eddies center position RMSE (km)

4.3 Comparison with state-of-the-art methods on a NATL60 OSSE

We are interested in comparing our estimations to state-of-the-art methods for gridding SSH maps. To this end, the Ocean Data Challenge 2020 (CLS/MEOM, 2020) provides a similar OSSE to the one we used, as well as the interpolations of several methods. The studied area is the same, and the included data are SSH, SST, surface currents and the simulated along tracks measures. However, the ground truth used is the NATL60 simulation (Ajayi et al., 2019) which uses the same physical model (NEMO 3.6) (Madec et al., 2017) but at finer scales than GLORYS, and without assimilation. Also, this simulation was run for only one year, which makes it difficult to train neural networks, this is why we designed our own OSSE. The state-of-the-art framework presented in this challenge is the following:

- DUACS: the operational linear optimal interpolation leveraging covariance matrix tuned on 25 years of data.
- DYMOST (Ubelmann et al., 2016; Ballarotta et al., 2020) and MIOST (Arduin et al., 2020) : two variants of the linear optimal interpolation where the Gaussian covariance model is changed for a non linear surface quasi-geostrophic dynamic model (for DYMOST) or by a wavelet base (MIOST).
- BFN (Le Guillou et al., 2020) : a data assimilation method that performs a back and forward nudging of a surface quasi-geostrophic model.

- 504 • 4DVarNet (Fablet et al., 2021): introduced 4DVarNet, a supervised deep learning
 505 framework. In this configuration, it only takes SSH observations as input.
 506 • MUSTI (Archambault et al., 2023): an unsupervised neural network that overfits
 507 SSH along tracks observations starting from an SST image. But this method must
 508 be refitted to new observations.

509 To produce our own estimation, we regrid the provided data to our resolution and
 510 perform the interpolation on this dataset without any finetuning or retraining. We eval-
 511 uate all methods on 42 days of simulation, (between October 22nd and December 2nd
 512 2012) which was the test set defined by the challenge. Each method is then evaluated
 513 using the following metrics, and we sum up the results in Table 7:

- 514 • μ and σ_t (in cm), are respectively the RMSE of the SSH and the temporal stan-
 515 dard deviation of this RMSE.
 516 • λ_x (in degrees) and λ_t (in days) are two spectral metrics, introduced by (Le Guil-
 517 lou et al., 2020). We compute respectively the spatial and temporal power spec-
 518 trum of the error, λ_x is then the smallest spatial wavelength where the power spec-
 519 trum of the error is equal to the power spectrum of the signal and λ_t its tempo-
 520 ral equivalent. For further information, we refer the reader to (Le Guillou et al.,
 521 2020)
 522 • μ_u and μ_v (in cm/s) are the RMSE between the geostrophic currents of the ground
 523 truth and the one of the estimation.

Method	SST	SUP	μ	σ_t	λ_x	λ_t	μ_u	μ_v
DUACS	✗	✗	4.89	3.02	1.42	12.08	16.8	16.2
DYMOST	✗	✗	5.18	3.05	1.35	11.87	16.8	16.8
MIOST	✗	✗	4.21	2.5	1.34	10.34	14.9	14.5
BFN	✗	✗	4.7	2.73	1.23	10.64	15.1	15.3
4DVarNet	✗	✓	3.26	1.73	0.84	7.95	13.1	12.8
MUSTI	✓	✗	3.12	1.32	1.23	4.14	12.2	14.2
SSH \mathcal{L}	✗	✓	3.75	2.0	1.21	8.74	13.3	13.5
SSH \mathcal{L}_{tri}	✗	✗	4.06	2.19	1.32	9.29	13.7	15.1
SSH \mathcal{L}_{tri_reg}	✗	✗	4.23	2.36	1.24	9.98	13.8	14.2
SSH+SST \mathcal{L}	✓	✓	2.88	1.24	0.95	4.51	11.4	11.4
SSH+SST \mathcal{L}_{tri}	✓	✗	3.08	1.41	1.18	5.18	11.8	12.8
SSH+SST \mathcal{L}_{tri_reg}	✓	✗	3.39	1.65	1.18	5.7	12.4	12.3

Table 7. Comparison of the state-of-the-art reconstruction methods on a 43-day OSSE. SST stands for whether or not the reconstruction methods are using SST, and SUP stands for whether or not the methods are supervised.

524 We clearly see in these scores a predominance of neural network-based methods (MUSTI,
 525 4DVarNet and ours) as the importance of the SST in the reconstruction (MUSTI, and ours).
 526 This analysis highlights the interest in using deep learning-based methods for these in-
 527 verse problems, as we can expect around 2 cm of error reduction on the operational in-
 528 terpolation scheme DUACS with our best method (41% of reduction). We also significantly
 529 reduce the errors on currents compared to DUACS's, by 5.7 cm/s for u and 5.4 cm/s for v
 530 (35% and 34% error reduction).

531 5 Conclusion and perspectives

532 5.1 Summary

533 Throughout this study, we show promising results for a neural interpolation of SSH
 534 tracks, even while training without fully gridded data. Leveraging an Observing System
 535 Simulation Experiment, we trained an attention-based auto-encoder neural network, with
 536 3 different loss functions (2 of them learning the reconstruction without ground truth),
 537 and using 3 sets of data (SSH only, SSH and noised SST, SSH, and SST). We show a sys-
 538 tematic improvement of the interpolation thanks to the use of SST as well for the SSH
 539 itself, but also for the reconstruction of currents and the detection of eddies. Using tem-
 540 perature data (noisy or not), the unsupervised inversion outperforms even the supervised
 541 SSH-only neural network (3.86 cm of RMSE for the unsupervised noisy SST against 4.18
 542 cm for the supervised SSH-only method). This shows the importance of contextual in-
 543 formation to constrain the inverse problem, even while learning with observation only.

544 Using AMEDA, an automatic eddy detection algorithm, we were able to identify
 545 cyclones and anticyclones in the ground truth and compare them with the eddies detected
 546 in the geostrophic approximation of the different mappings. This allows a deeper phys-
 547 ical interpretation than the SSH reconstruction alone. We conclude that SST aids in cap-
 548 turing finer structures that might be overlooked by SSH-only methods, but also that the
 549 key physical properties of the detected eddies such as size, speed, or center position are
 550 better rendered by SST-using methods. Furthermore, when it comes to unsupervised re-
 551 construction, we show that the non-regularized and regularized inversions have close de-
 552 tection scores, but their errors are different. The regularized inversions exhibited lower
 553 recall scores, indicating that certain eddies were not detected due to the regularization
 554 process. However, they demonstrated higher precision scores, implying increased con-
 555 fidence in the eddies that were successfully detected.

556 We conducted an evaluation of our model’s performance by comparing it with state-
 557 of-the-art interpolation techniques produced during the Ocean Data Challenge 2020 which
 558 provided diverse input data, ground truth measurements, and mappings derived from
 559 different methods. Remarkably, our approach exhibits superior performance even with-
 560 out retraining the neural network on this novel dataset, thanks to the integration of SST
 561 information. Notably, the utilization of SST led to a substantial enhancement of 41%
 562 in terms of RMSE for SSH when compared to the widely used L4 product from DUACS.
 563 Moreover, we observed significant improvements of 34% and 35% for u and v currents,
 564 respectively. These findings present promising perspectives for advancing satellite SSH
 565 gridding through the application of deep learning methodologies and the fusion of di-
 566 verse physical information.

567 5.2 Perspectives

568 **Transfer to real-world data.** In this work, we performed SSH interpolation on
 569 an OSSE, which allows us to evaluate our methods on an idealized simulation of satel-
 570 lite tracks. The OSSE has the advantage of being more interpretable than real-world data,
 571 as the ground truth is accessible for performance evaluation, but is less realistic, espe-
 572 cially in the simulation of SST noise which is hard to model. While simulations provide
 573 valuable insights, their direct application to real-world observations can be challenging
 574 due to inherent differences between the two domains. However, by employing transfer
 575 learning, we expect to leverage the knowledge gained from simulations to enhance re-
 576 construction algorithms for real-world data. In further work, we are interested in com-
 577 paring strategies able to learn directly from observations such as (Archambault et al.,
 578 2023; S. A. Martin et al., 2023), and a network that would benefit from supervised pre-
 579 training on simulation, and transfer on real-world observations. For instance, a model
 580 supervised on a simulation can be adapted to the new domain using one of the unsuper-

581 vised losses used in this study. This will require accurate modeling of the SST input noise
582 and an adapted transfer strategy in order for the pre-training to be efficient.

583 **Global interpolation.** Furthermore, to get toward a global gridded SSH prod-
584 uct, many challenges still need to be addressed. For instance, as the geostrophic equi-
585 librium depends on the Coriolis force surface projection, and thus on the latitude con-
586 sidered, we may require a model to be trained on several areas with different latitudes.
587 Also, we can wonder which strategy is more efficient between training a global model or
588 several local models, each one specialized for a range of latitude or geographical area.
589 Closed seas and coastal water also have very different physical interactions and should
590 be reconstructed by different methods.

591 **Using different input and output data.** We have demonstrated the benefit of
592 using multi-physical information, specifically SST, to enhance SSH reconstruction through
593 the implementation of a flexible neural network framework. The integration of data from
594 diverse physical sources exhibits promising outcomes, yet conventional model-based meth-
595 ods encounter challenges due to noise and observational difficulties associated with real-
596 world data. In contrast, machine learning opens doors to augment these methods with
597 diverse and abundant data sources. For instance, in our investigation, we employed noisy
598 yet complete SST data, but using L3 SST products is also possible. Furthermore, an in-
599 triguining prospect arises as to whether Level 4 (L4) and Level 3 (L3) SST products can
600 be effectively combined, thereby potentially yielding even more precise and exhaustive
601 information. Other physical measures might improve the reconstruction, such as chloro-
602 phyll maps that track plankton advected by currents (Kahru et al., 2012).

603 Data availability statement

604 The GLORYS data (CMEMS, 2020) that we used as a reference throughout this
605 study are freely available and distributed by the European Union-Copernicus Marine Ser-
606 vice (<https://doi.org/10.48670/moi-00021>). The L3 altimeter (CMEMS, 2021) mea-
607 sures used to retrieve along tracks coordinates and the L3 SST measures (CMEMS, 2023)
608 used to compute a realistic cloud cover are distributed by the same service (with doi <https://doi.org/10.48670/MOI-00146> and <https://doi.org/10.48670/MOI-00164> respectively).

610 The data of the Ocean Data Challenge 2020 OSSE (ground truth, inputs, and base-
611 lines) are available at <https://doi.org/10.24400/527896/A01-2020.002> and were de-
612 veloped, validated by CLS and MEOM Team from IGE (CNRS-UGA-IRD-G-INP), France
613 and distributed by Aviso+.

614 The preprocessed data and the weights of our neural networks are available here: <https://doi.org/10.5281/zenodo.8380281> and our code is hosted on the following repository:
615 <https://gitlab.lip6.fr/archambault/james.2023>
616

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620 Le Vu, and Evangelos Moschos, for their useful advice and assistance with the OSSE de-
621 sign and the automatic eddy detection algorithm AMEDA.

622 6 Annexes

623 6.1 Along-track spatial derivative

624 To calculate the first and second spatial derivatives of the SSH along the ground
625 tracks which we use to regularize the network (see Section 3.3). Given \mathbf{Y}^{ssh} , we approx-

626 imate the derivative by the rate of change of the SSH:

$$\frac{\partial}{\partial s} \mathbf{Y}_i^{ssh} \simeq \frac{\mathbf{Y}_{i+1}^{ssh} - \mathbf{Y}_i^{ssh}}{\Delta s} \quad (9)$$

627

$$\frac{\partial^2}{\partial s^2} \mathbf{Y}_i^{ssh} \simeq \frac{\frac{\partial}{\partial s} \mathbf{Y}_{i+1}^{ssh} - \frac{\partial}{\partial s} \mathbf{Y}_i^{ssh}}{\Delta s} \quad (10)$$

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where Δs is the ground distance between the measures. We only compute the spatial derivatives from observations coming from the same satellite and only if the measures are taken with less than two seconds of delay. This way we estimate spatial derivatives only where the rate of change is a valid approximation of the derivation.

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6.2 Detection plot

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In the following, we present the Ensemble interpolation of the methods for three days. To select which day to look at, we computed the daily error of the SSH method and the SSH+SST error. The first day is chosen so that the gap between these two errors is maximal (the SST method performs a lot better than the SSH-only method). The second day corresponds to the median error gap, and the last to the minimal error gap. With the reconstructions of every method and the corresponding SSH ground truth, we also provide the SST and the noised SST. To highlight the eddy signatures in SST data we plot the ground truth eddy computed on SSH on SST images as well.

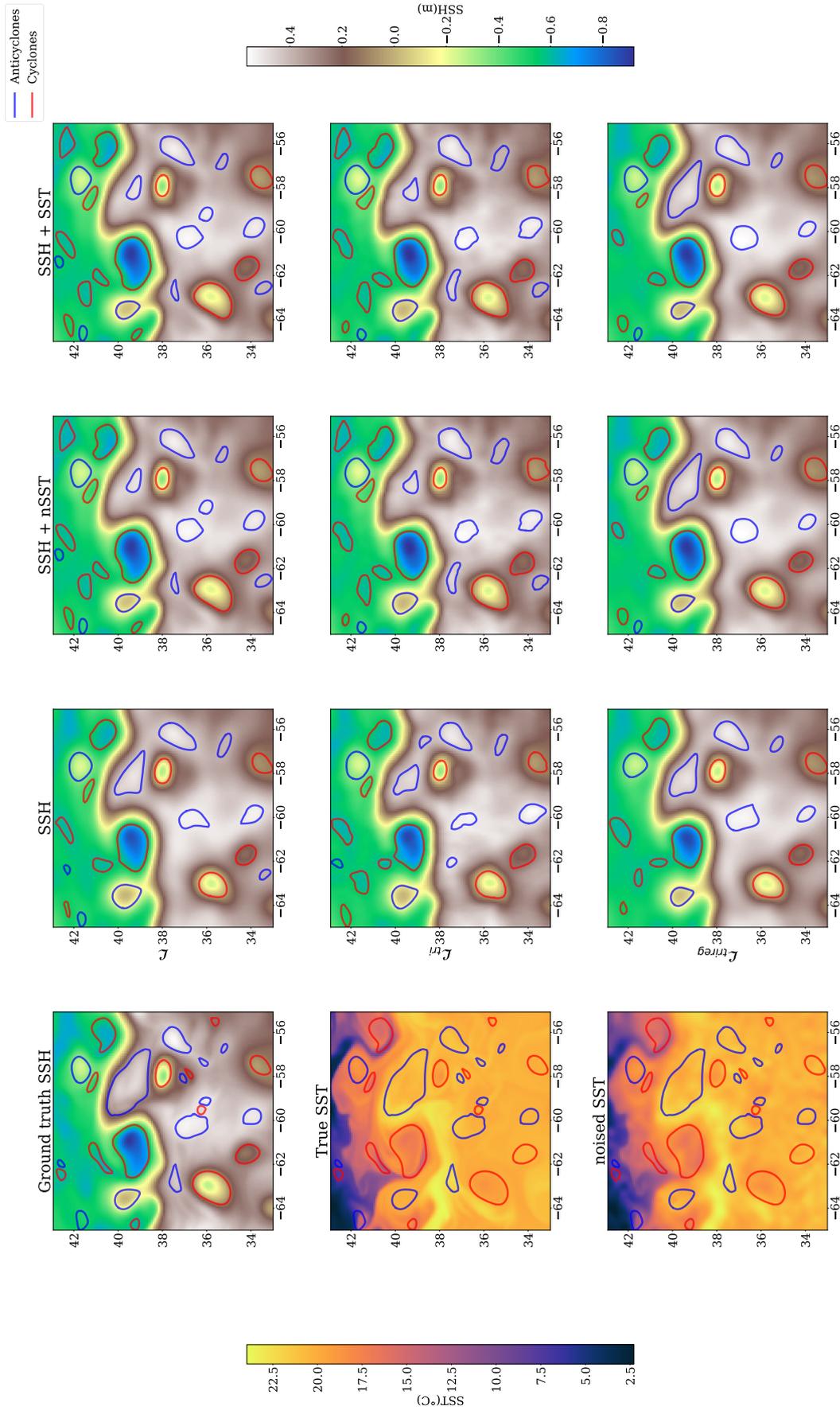


Figure 7. Eddy detection on the day of maximal error gap between SSH-only method and SST method. It corresponds to February the 7th 2017

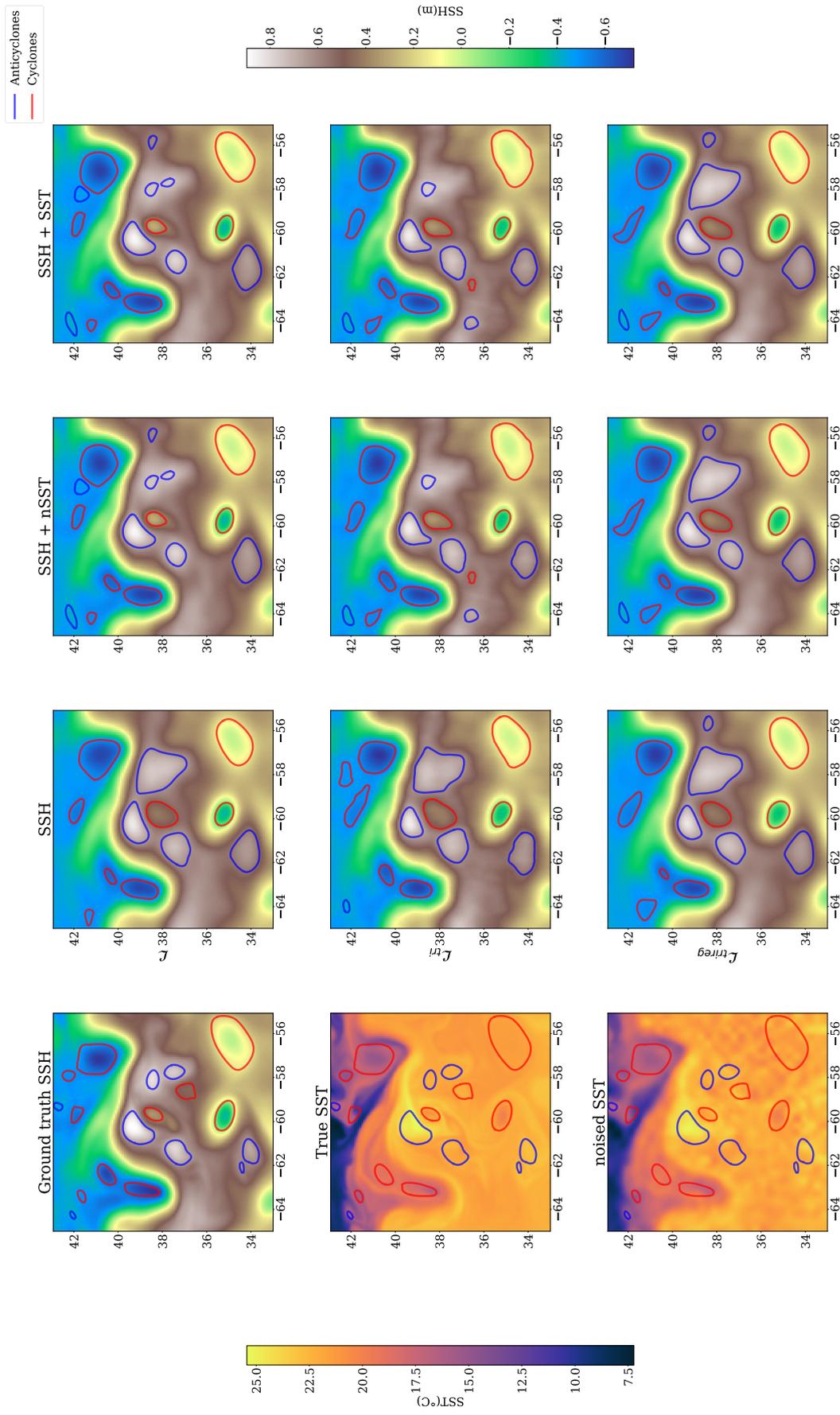


Figure 8. Eddy detection on the day of median error gap between SSH-only method and SST method. It corresponds to December the 20th 2017

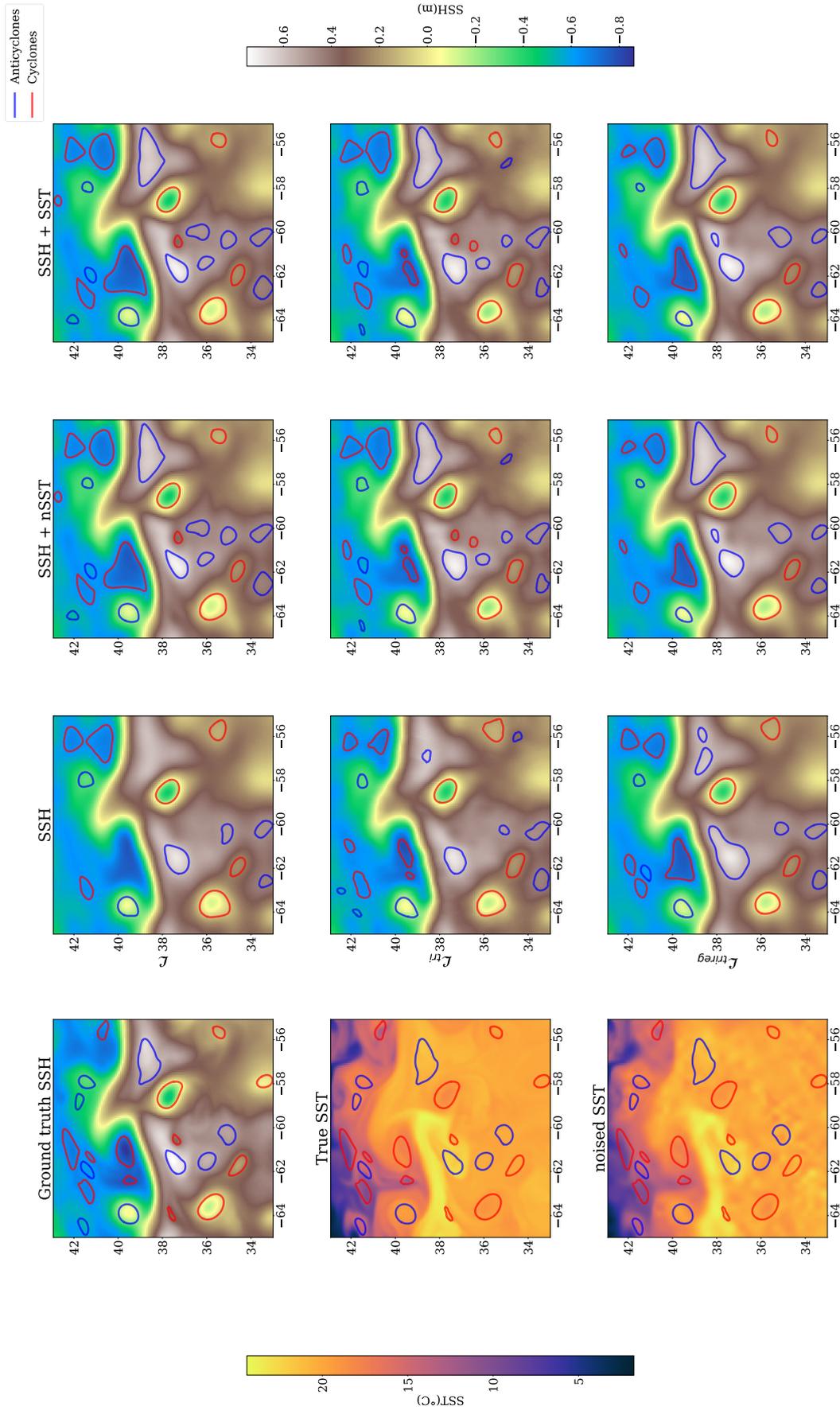


Figure 9. Eddy detection on the day of min error gap between SSH-only method and SST method. It corresponds to February the 15th 2017

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