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State estimation of surface and deep flows from sparse SSH observations of geostrophic ocean turbulence using Deep Learning

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Key Points:

- Deep Learning framework is developed for temporal SSH interpolation in a baroclinically unstable current
- Residual Neural Networks outperform linear and dynamical SSH interpolation techniques.
- Skillful estimation of unobserved deep flows from temporally-sparse SSH observations is plausible

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Abstract

Satellite altimeters provide global observations of sea surface height (SSH) and present a unique dataset for advancing our theoretical understanding of upper ocean dynamics and monitoring its variability. Considering that mesoscale and submesoscale SSH patterns can evolve on timescales comparable to or shorter than satellite return periods, currently available altimetry observations are still spatially and temporally sparse and hence it is challenging to accurately reconstruct continuous SSH evolution. Here we explore the possibility of SSH interpolation using Deep Learning — a machine learning approach that extracts information only from data. Using synthetic observations taken from an idealized quasi-geostrophic model of baroclinic ocean turbulence, we demonstrate that Convolutional Neural Networks with Residual Learning are superior in SSH reconstruction than the linear and recently developed dynamical interpolation techniques. Furthermore, the neural network can provide an accurate state estimate of unobserved deep ocean currents at mesoscales, suggesting that SSH patterns of eddies do contain substantial information about ocean interior that is necessary for SSH prediction. Our framework is highly idealized and several crucial improvements such as transfer learning and diversification of training data would be necessary to implement before its ultimate use with real satellite observations. Nonetheless, by providing a proof of concept, our results point to Deep Learning as a viable alternative to existing interpolation and more generally state estimation methods for satellite observations of baroclinic ocean turbulence.

Plain Language Summary

Satellite sea surface height (SSH) observations provide critical insights into the variability of ocean currents. However, these observations are spatially and temporally sparse, presenting a challenge for reconstructing time-continuous SSH maps particularly at resolutions containing relatively fast-evolving upper-ocean eddies. Further limitations are due to the fact that the evolution of SSH is not self-contained as it is affected by unobserved deep ocean flows. In this study, we test a different approach to address poor temporal sampling of SSH: a machine learning framework that relies on pattern recognition in large-scale ocean turbulence. We demonstrate that deep artificial neural networks can generate a skillful state estimation of unobserved deep ocean currents and outperform conventional SSH reconstruction methods in an idealized model of ocean turbulence. In providing the proof of concept, our results strongly point at Deep Learning learning as a viable alternative to existing interpolation and state estimation methods for satellite oceanography.

1 Introduction

Satellite-derived global observations of sea surface height (SSH) has shed light on many dynamical processes including large-scale circulation, propagation of waves as well as on the evolution of the mesoscale eddy field (Chelton et al., 2011; Fu et al., 2010). Since the satellite era, an increasing amount of evidence points towards the mesoscale eddies being a key component of the global ocean circulation and significantly impact, among others, carbon sequestration, biological productivity, heat transport and thus the Earth’s climate as a whole (Ferrari & Wunsch, 2009). Nonetheless, understanding and monitoring oceanic energy spectrum and associated spectral energy fluxes (Scott & Arbic, 2007; Aluie et al., 2018), understanding tracer dispersion (Abernathy & Marshall, 2013) or inferring subsurface flows (Klein et al., 2009) still remains challenging because these quantities depend on higher-order SSH derivatives and hence require high resolution and accuracy. The regularly-gridded SSH data, e.g. AVISO (Ducet et al., 2000), is spatially and temporally interpolated from along-track altimetry measurement using objective mapping and hence its accuracy is constrained by the density of observations and by the deficiencies of the interpolation technique. To provide better coverage, several altimeters have been put in orbit but their 10-20 days repeat orbits and relatively coarse along-track resolutions allow to view the ocean dynamics only down to relatively large mesoscale eddies (Wunsch, 2010).

The upcoming Surface Water Ocean Topography (SWOT) altimeter mission (Fu & Ubelmann, 2014) promises to observe ocean mesoscale eddies and submesoscale fronts (50 km) at unprecedented spatial resolutions, potentially resolving 15-30km wavelengths. However, the temporal resolution of the altimeter (i.e., a complete repeat cycle of 21 days) is not sufficient to continuously capture the evolution of submesoscale eddies and fronts. The mismatch between the high spatial resolution and the moderate temporal resolution presents a challenge for reconstructing time-continuous maps of SSH. This task is especially challenging in eddy-rich regions where small-scale SSH anomalies can evolve relatively fast compare to satellite return periods, e.g. in the Antarctic Circumpolar Current, the Kuroshio Extension and the Gulf Stream, all of which are key players in the climate system. It is thus crucial to develop frameworks to efficiently extract information about oceanic eddy dynamics from the spatially and temporally sparse SSH observations.

1.1 SSH interpolation and associated dynamical limitations

Spatiotemporal interpolation or gridding of SSH data is inherently linked to ocean physics as the success of a given technique ultimately should rely on the pertinence of its assumed model (either dynamical or statistical) that captures the essence of eddy propagation in space and time. To illustrate this point, imagine a coherent moving eddy in a turbulent field and several altimeter tracks passing through it at different times and directions: if there is an accurate model of eddy propagation, it would allow to pinpoint only those tracks that have passed over this specific eddy and combine this information to constrain the two-dimensional eddy shape. Thus, without a model of eddy evolution, or more generally SSH evolution, the information from various altimetry tracks could not be used in an optimal way. However, due to the stratified nature of geostrophic ocean turbulence, the unobserved subsurface flows can affect surface dynamics and hence the knowledge of the SSH field may not be self-sufficient to infer its evolution. Given the lack of subsurface information at eddy scales, constructing a reduced self-contained model of SSH evolution is challenging.

Existing methods for spatiotemporal SSH interpolation can be broadly split into two distinct classes: methods that rely on a postulated dynamical model of SSH evolution and purely data-driven methods, both having their advantages and disadvantages. To avoid prescribing a dynamical model, statistical models relying on data only, e.g. objective interpolation methods (Davis, 1985; Le Traon et al., 1998; Ducet et al., 2000). Their premise is to incorporate spatiotemporal correlations and measurement error into a statistical model that provides the most likely estimate of the true continuous state, given available observations.

149 the discarded term was the only one that depended on the unknown streamfunction, ψ_2 , it
 150 is possible to integrate the approximate PV-conservation equation forward and backward
 151 in time given only ψ_1 observations, as was done in Ubelmann et al. (2015). Even though
 152 in many ocean regions both deep and upper-ocean currents are dynamically active, recon-
 153 structing SSH using the dynamical interpolation technique performed well, being superior
 154 to linear interpolation methods because it relied, at least approximately, on the fundamen-
 155 tal PV-conservation constraint. Nonetheless, the dynamical interpolation method can lead
 156 to significant errors (see Results), implying that the omitted term, while being relatively
 157 small, can substantially impact SSH evolution on timescales comparable to return periods
 158 of altimetry satellites.

159 1.2 Rationale for Deep Learning approach.

160 A clear way of improving the dynamical interpolation algorithm would be to include
 161 the contribution of the barotropic mode to SSH evolution. However, comprehensive mea-
 162 surements of deep ocean currents at eddy scales are missing, posing a significant challenge of
 163 inferring them from only SSH observations. Without taking into consideration the physical
 164 processes that have lead to the generation of any given SSH snapshot, there is a wide range
 165 of plausible ways in which ψ_1 could be decomposed into baroclinic and barotropic modes,
 166 each corresponding to the distinct configuration of PV anomalies in the two layers. How-
 167 ever, considering that PV anomalies are specifically due to baroclinic instabilities and they
 168 obey specific conservation laws (Eq. 1), the barotropic and baroclinic modes are inherently
 169 entangled and this must provide at least partial constraints on how any specific SSH pattern
 170 could be partitioned. Since the QG model exhibits highly non-linear and chaotic behavior,
 171 an analytical approach to disentangle the modes has not been found but the evidence that
 172 data-driven approach might be relevant has been presented in the literature. In particu-
 173 lar, mooring observations demonstrate that surface and subsurface flows are significantly
 174 correlated such that a single empirical orthogonal function (EOF) can explain a signifi-
 175 cant amount of variance of the overall vertical velocity profile Wunsch (1997); de La Lama
 176 et al. (2016). Furthermore, machine learning techniques such as self-organizing Chapman
 177 & Charantonis (2017), as well as convolutional neural networks (Bolton & Zanna, 2019),
 178 have been used to estimate subsurface flows from SSH data. However, the unknown term
 179 $D\psi_2 = D_t(\psi_2 + \mathbf{u}_1 \cdot \nabla \psi_2)$ in Eq. 1 can only provide a substantial contribution to the PV
 180 budget if $D\psi_2$ has a substantial component that is decorrelated from ψ_1 because $\mathbf{u}_1 \cdot \nabla \psi_1 = 0$,
 181 and $D\psi_2 \ll D\psi_1$ for surface-amplified flows. Thus the key for a more accurate SSH in-
 182 terpolation lies in estimating the component of ψ_2 that is decorrelated from ψ_1 – a problem
 183 that is tightly linked to estimating eddy heat fluxes in baroclinically unstable flows. Us-
 184 ing residual neural networks, George et al. (2019, under review) have demonstrated that
 185 ψ_1 indeed contains substantial information about the decorrelated part of the subsurface
 186 streamfunction ψ_2 , allowing to estimate about 60% of the variance in eddy heat fluxes only
 187 from SSH snapshots. Given that machine learning methods can extract information from
 188 SSH patterns to estimate the component of $D\psi_2$ that is uncorrelated with ψ_1 when esti-
 189 mating the eddy heat fluxes, here we hypothesize that machine learning techniques could
 190 outperform the dynamical interpolation methods.

191 2 Methods

192 Here we present a machine learning framework that mimics the task of dynamical inter-
 193 polation, i.e. reconstructs the SSH snapshot that occurred between two given SSH snapshots
 194 separated by 20 days (Ubelmann et al., 2015). We use machine learning as a tool to shortcut
 195 the formal process of data assimilation and to establish if there are substantial possible con-
 196 nections between the dynamical evolution of eddies and spatiotemporal interpolation. We
 197 are interested in providing a proof-of-concept machine learning framework and understand-
 198 ing its dynamical limitations, i.e. those that are not subject to insufficiency or poor quality
 199 of data. We develop and test our method in an idealized framework of predicting SSH snap-

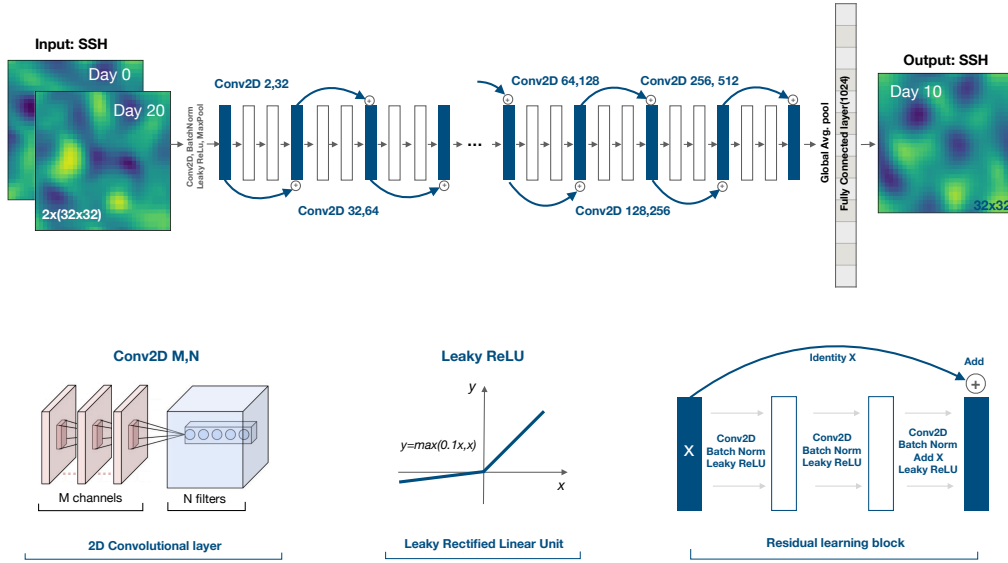


Figure 1. Architecture of the Deep Learning neural network with residual learning (slightly modified from the well-known ResNet50 architecture He et al. (2016)). The input consists of two SSH snapshots separated by 20 days (in case of SSH input with missing data, those values are set to zero). A set of convolutional layers are then applied to create abstract representation of the input patterns in a bottleneck fashion: when image sizes decrease by a factor of two, the number of filters increase by a factor of two. Each convolutional layer is followed by the batch normalization and the application of the nonlinear function (Leaky Rectified Linear Unit). Residual learning blocks are saving the information from one layer and adding its identity to the output several layers ahead. The output from the convolutional layer is subject to global average pooling and flattening into a vector that is finally densely connected to the output.

shots that were generated by a quasigeostrophic (QG) model of baroclinically unstable flow. We find the QG model to be optimal for our goals as is pertinent to many energetic regions in the ocean while being relatively simple that a large volume of data can be generated for training and testing; furthermore, the model allows us to directly benchmark machine learning against the dynamical interpolation technique that also utilizes QG dynamics. Below we describe our neural network architecture for spatiotemporal SSH interpolation and the QG model used for the generation of training and testing datasets.

2.1 Deep Learning framework: Residual Convolutional Neural Networks

Artificial neural networks are based on the idea of approximating the ‘output’ by taking the ‘input’ variable and performing a large number of matrix additions and multiplications, applying non-linearity functions, and either condensing or expanding the variable dimension as it passes from layer to layer. The resulting network contains a large number of free parameters that are later adjusted to optimize a given loss function, commonly taken as a measure of difference between the prediction and the truth. Because we are trying to extract information from eddy patterns expressed in SSH fields, the choice of convolutional neural networks (CNNs) is rationalized. In passing information from layer to layer, CNNs define a set of filters (kernel matrices with prescribed dimensions) and convolve images

217 to produce more abstract levels of information that is passed on to the next layer. Here
 218 we implement the ResNet50 architecture – a Convolutional Neural Network with Residual
 219 Learning blocks (He et al., 2016). The Residual Learning is a process by which the infor-
 220 mation is not only transferred sequentially from one layer to another but is also transferred
 221 via skip connections that add the identify of the current layer to the layer that is a few
 222 ahead (see Fig. 1); the presence of skip connections can result in better performance for a
 223 wide range of computer vision problems (Targ et al., 2016). We note that we have explored
 224 several simpler architectures like shallow neural networks with only dense connections, and
 225 simpler VGG-type architectures without residual learning but have achieved significantly
 226 poorer performance; we thus present the network architecture that have lead to a signifi-
 227 cant skill, although there is always a possibility that superior neural network architectures
 228 may exist. The graph of the architecture used in this study, outlining all hyperparam-
 229 eters together with the Python code of its implementation in Tensorflow/Keras as well
 230 as the training datasets can be found here https://drive.google.com/drive/folders/1tZrplLw2m19CB1YcQABj6pn0a7_-H63n?usp=sharing.
 231

232 As a performance metric we define the model skill that is proportional to the loss
 233 function and normalized by the standard deviation of the SSH signal in the following way:

$$234 \quad Skill = 1 - \frac{\sqrt{\overline{SSH_{predicted} - SSH_{true}}^2}}{\sqrt{\overline{SSH_{true}}^2}}; \quad (3)$$

235 For reference, the maximum skill=1 is achieved when the predicted and true images are
 236 exactly the same; the skill=0 corresponds to a prediction that makes the same error as
 237 assuming a spatially homogeneous SSH field, and negative skill implies an even worst fit.
 238 This definition of skill is more conservative than the correlation coefficient or R-squared
 239 value; for example, ρ_2 is correlated to ρ_1 with an average correlation coefficient of 0.74 and
 240 the linear regression model has R-squared of about 0.55 but the skill of only 0.33 if defined
 241 as in equation 3 above. It is thus important to compare results from different publications
 242 using consistent metrics. Here we stick with the skill metric that is based on the RMS-error
 243 normalized by the standard deviation as it is a natural choice for a neural network loss
 244 function to minimize during training.

245 Coefficients of filter matrices, along with all other weights and biases involved in the neu-
 246 ral network architecture are then iteratively optimized using the Adam optimizer (Kingma
 247 & Ba, 2014) to minimize the loss function that is the root-mean-square difference between
 248 the predicted and true SSH images (or equivalently to maximize the skill). The parameter
 249 optimization procedure requires evaluating neural network predictions for a large volume of
 250 training data and hence the final optimized state of a particular neural network depends only
 251 on the training data itself. To test if a general dependence was found the neural network
 252 skill is estimated for a group of three independent datasets: training, validation, and testing
 253 sets. Training data is used only for training purposes, validation data is used to evaluate
 254 the skill of the neural network and to identify a stoppage criterion for the training, while
 255 the test data is used at the very last step to define the skill of a trained neural network. All
 256 three datasets were generated from different numerical simulations to ensure that overfitting
 257 didn't occur and that a general law was found.

258 **2.2 Synthetic training data: quasigeostrophic model**

259 Deep neural networks typically require a large volume of training data to identify a
 260 general law. In the absence of high-quality or sufficiently large volume of data neural
 261 networks are likely to overfit the training data and have poor skill when evaluated on the test
 262 data. To avoid these issues we choose to train neural network on synthetic data generated
 263 using an idealized model of ocean turbulence – the two layer quasigeostrophic (QG) model
 264 (Phillips, 1951; Vallis, 2017). The QG model is pertinent to baroclinically unstable flow
 265 and contains the propagation dynamics of large-scale ocean eddies, including advection by
 266 mean flow, beta drift, and eddy interactions with mean flow. Our choice of using the

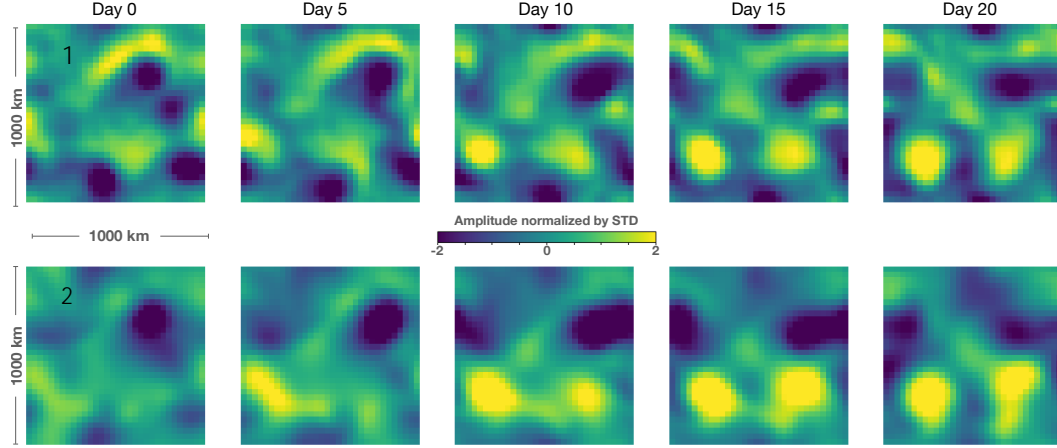


Figure 2. An example of the eddy field evolution over the course of 20 days as generated by the QG model of a baroclinically unstable current. Top panels show surface streamfunction ψ_1 (or SSH) and bottom panels show the corresponding deep ocean streamfunction ψ_2 , both being normalized by their respective standard deviations; domain size is 1000x1000 km and rows correspond to streamfunction snapshots taken 5 days apart. Note that the eddy field dramatically changes over the course of 20 days (SSH decorrelation time scale is about 10–20 days), implying that conventional linear or optimal interpolation methods would lead to significant errors if available observations are separated by more than the decorrelation timescale.

267 two-layer model is rationalized because i) ocean currents are predominantly composed of
 268 the barotropic and the first baroclinic mode (Wunsch, 1997; Smith & Vallis, 2001) and ii)
 269 it is the minimal model demonstrating the difficulty of predicting SSH evolution without
 270 direct observations of subsurface flows because both layers necessarily are dynamically active
 271 during baroclinic instabilities, and iii) the dynamical interpolation method also relies on QG
 272 dynamics which allows to make a fair performance comparison.

273 The quasigeostrophic model relies on the conservation of potential vorticity and sim-
 274 ulates mesoscale turbulence driven by baroclinic instabilities associated with the vertical
 275 shear of mean flow, requiring a minimum of two vertically stacked shallow layers. The con-
 276 servation laws for the top and bottom layer potential vorticities, $q_{1,2}$, are written in the
 277 following way:

$$278 \quad \frac{Dq_1}{Dt} = \frac{D}{Dt} [r^{-2} \psi_1 + \frac{f_0^2}{g^0 H_1} (\psi_1 - \psi_2) + y] = 0 \quad (4)$$

$$279 \quad \frac{Dq_2}{Dt} = \frac{D}{Dt} [r^{-2} \psi_2 + \frac{f_0^2}{g^0 H_2} (\psi_2 - \psi_1) + y] = r_{EK} r^{-2} \psi_2; \quad (5)$$

280 where $\psi_{1,2}$ is the top and bottom layer streamfunctions, f_0 is the Coriolis parameter and
 281 ψ is its derivative in the meridional y -direction, g^0 is the reduced gravity, $D=D_t = \partial_t +$
 282 $\mathbf{u} \cdot \nabla$ is the material derivative using corresponding layer' geostrophic velocity \mathbf{u} , and r_{EK}
 283 is the bottom drag coefficient. The relative importance of the discarded term in the PV-
 284 conservation budget in Eq. 1, $D_{bt} = D_t$, could be estimated by comparing its magnitude
 285 to $D_{t1} = D_t$, where both material derivatives use velocity in the top layer. The ratio of
 286 these terms would scale roughly as the ratio of characteristic amplitudes of the barotropic
 287 and surface streamfunctions, which we find from numerical simulations to scale as the ratio
 288 of layer depths in QG simulations of baroclinic instabilities, i.e. $[\frac{-2}{b;t} = \frac{-2}{1}]^{\frac{1}{2}} \sim O(H_1 = H_2)$.
 289 Since in most ocean regions the pycnocline is relatively shallow compared to the full depth
 290 of the ocean, the flows are surface-amplified and the discarded term is relatively small but

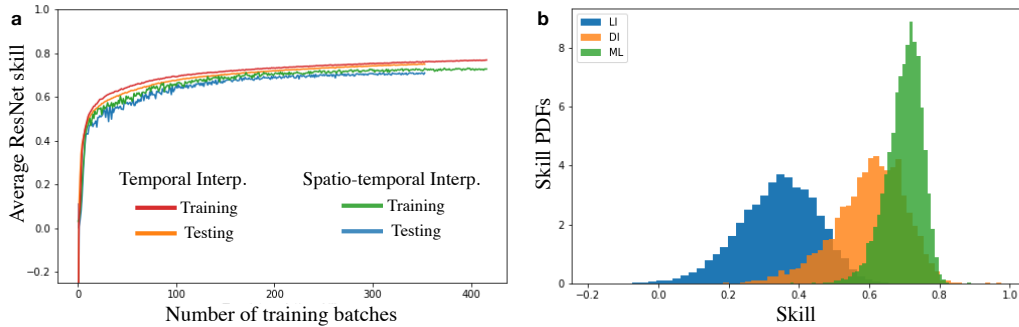


Figure 3. a) The evolution of the ResNet50 model skill during its training; 10 training mini-batches correspond to one epoch, while the actual number of batches is 128 and the total number of samples used in training is about 80,000; testing was conducted on 10,000 samples. b) comparison of skill distributions of the linear interpolation (LI), dynamical interpolation (DI), and the machine learning method evaluated on the test data set. Note that the lack of skills close to 1 hint at the existence of a dynamical barrier for SSH interpolation likely due to the chaotic nature of QG equations; i.e. the information content about the predicted SSH image is decreasing with the increased amount of time separation between the input image as the phase space trajectories are being mixed to the point where the dependence of initial conditions is being lost.

291 non-negligible and can substantially impact the SSH evolution leading to significant errors
 292 of the dynamical interpolation (see Results).

293 The QG model has been configured to represent baroclinically unstable mid-latitude
 294 currents such as the Gulf Stream or Kuroshio. Model parameters are as follows: the Rossby
 295 deformation radius is 40 km, the ratio of mean layer depths is 0.2, there is a steady uni-
 296 form mean vertical shear of 0.2 m/s, beta plain parameter corresponds to a latitude of
 297 40 degrees, linear Ekman friction was prescribed in the bottom layer for dissipation, and
 298 high-wavenumber motions are being filtered in Fourier space for all variables (more details
 299 could be found in Flierl (1978); Arbic et al. (2012)). The QG model is integrated forward in
 300 time using an ensemble of noisy initial conditions to produce a large volume of data: about
 301 100,000 SSH snapshots separated by 10 days (Figure 2). Over a timescale of 20 days, SSH
 302 fields become substantially decorrelated such that it is hard to identify any persisting eddies
 303 because their shapes and intensities have been dramatically changed due to interactions
 304 with other eddies (Figure 2). We ensure that the data for training/validation/testing comes
 305 from distinct simulations to accurately access the generalization skill of the neural network.

306 **3 Results**

307 **3.1 Spatiotemporal SSH interpolation**

308 Two separate neural networks were trained to perform two types of interpolation tasks
 309 to identify SSH field: i) temporal interpolation where the input consists of two SSH snap-
 310 shots separated by 20 days, and ii) spatiotemporal interpolation with the same input as
 311 for the temporal interpolation but with SSH images having missing data. For the temporal
 312 separation of SSH images we chose 20 days because it is of the order of the return periods
 313 for existing altimeters and to be consistent with Ubelmann et al. (2015). For the spatioten-
 314 temporal interpolation, we choose the area of missing data to roughly correspond to that of
 315 the SWOT observations over its return period. For a 1000 km domain, SWOT would have

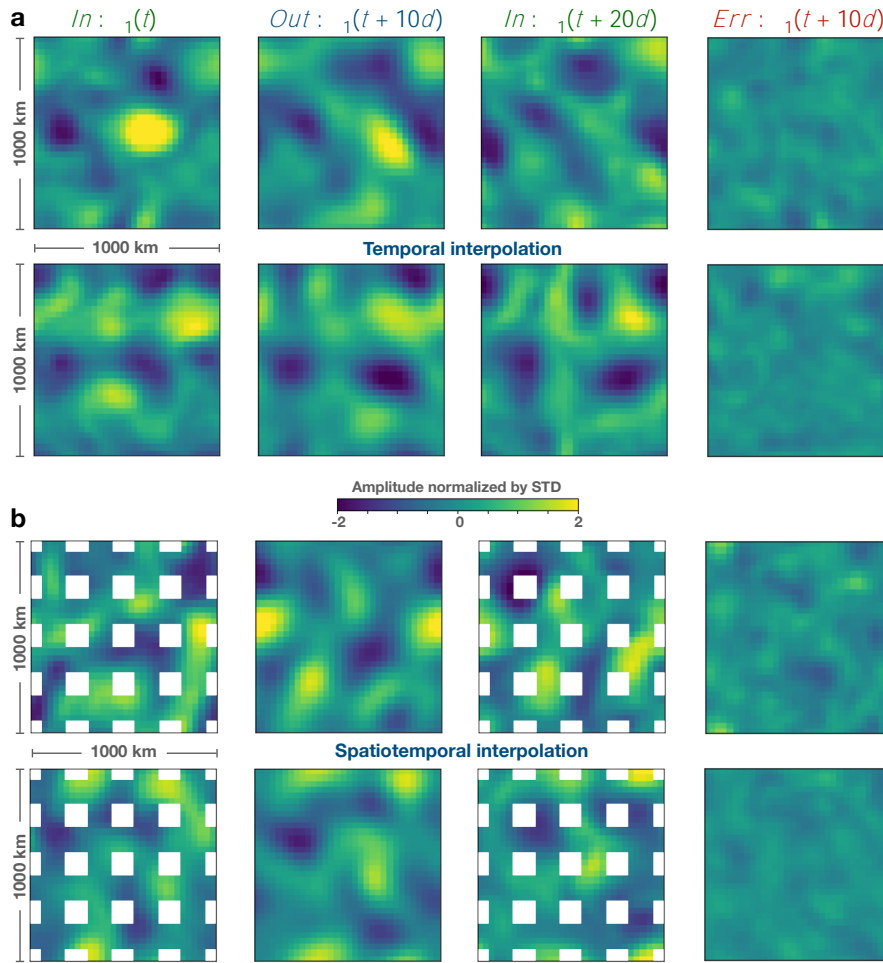


Figure 4. Examples of temporal (a) and spatiotemporal (b) interpolation of SSH data using the Deep Learning framework. Each row represents a randomly chosen interpolation example from the testing dataset (for a statistical distribution of prediction skill see Figure 3). The input SSH fields, $\eta_1(t)$ and $\eta_1(t+20d)$ are separated by 20 days and plotted in the first and the third columns correspondingly, while the predicted SSH field at day 10 ($\eta_1(t+10d)$) is plotted in the second column; the prediction error is plotted in the fourth column. White regions in the case of spatiotemporal interpolation denote areas of missing data. Domain size for both input and prediction is 1000km by 1000km. SSH data for training and testing was generated using baroclinically unstable QG model of ocean turbulence with configuration pertinent to midlatitude ocean jets (see Methods).

316 about four crossings (each having a swath of 120 km) with one inclination angle and another
 317 four with an opposite angle (see e.g. Figure 1 in Gaultier et al. (2016)). While SWOT would
 318 have missing-data areas in the shape of a rhombus, here for simplicity we have prescribed
 319 square shapes as there is no reason to assume this would lose any generality.

320 The neural networks were trained using about 100K data samples, both achieving a sig-
 321 nificant performance skill and producing realistic SSH images with small errors (see Figure
 322 4). The average prediction skill for both simulations plateaued at about 0.7 and it wasn't
 323 significantly smaller when evaluated on the test dataset (Figure 3 a), implying that a gen-
 324 eralized dependence has been found. A few illustrative examples of eddy field evolution are
 325 shown in Figure 4a, demonstrating the non-trivial SSH evolution that occurs in a chaotic

326 QG model of baroclinically unstable flow. In the top-row example of Figure 4a, the strong
 327 positive SSH anomaly in the center of the domain almost completely disappeared after 20
 328 days, yet the neural network was still capable to reconstruct the SSH state at day 10. For
 329 such examples when the eddy field changes dramatically with time, linear or objective in-
 330 terpolation techniques perform poorly as they do not rely on any dynamical model of SSH
 331 evolution and only make use of autocorrelation as a statistical model. Evaluated on a large
 332 number of testing data (10K samples), the machine learning model outperformed the linear
 333 and dynamical interpolation techniques, having not only a better average skill but also much
 334 more infrequent occurrence of low-skill interpolations, i.e. much narrower skill-distribution
 335 tail in the direction of small skills (Figure 3b). Noticeably, the linear interpolation skill can
 336 be so low that it has values reaching zero, i.e. its prediction is no better than assuming that
 337 $SSH = 0$ everywhere in the domain. The dynamical interpolation is much better than that
 338 but still has a significant probability of poor interpolations in the skill range of about 0.4-0.6.
 339 While the machine learning technique is superior to other methods, it is important to note
 340 that it still does not provide a perfect reconstruction and has a limit in skill abounded by
 341 about 0.8. Since we are utilizing only surface observations while SSH evolution depends also
 342 on the unknown subsurface flow, it is, of course, expected that the interpolation skill would
 343 not be perfect: it is inherently a partial information problem. In addition to having partial
 344 observations, the chaotic nature of the flow also must be contributing to the skill limitation:
 345 if the SSH images are separated by a sufficiently large amount of time (greater than the
 346 characteristic Lyapunov exponent timescale), there should be no physical or statistical rela-
 347 tionship between them and no interpolation technique could have a skill significantly above
 348 zero. Yet, the 20-day separation timescale, which is of the order of the return periods for
 349 existing altimeters, still allows one to extract sufficient information even for highly energetic
 350 baroclinically unstable flows.

351 3.2 State estimation of unobserved deep ocean flows at mesoscales

352 Here we assess the efficacy of the Deep Learning framework in addressing the state
 353 estimation problem, i.e. estimating all dynamical variables in the ocean turbulence model,
 354 which in our case of a two layer QG model implies estimating both surface and subsurface
 355 layer streamfunctions. Conventionally, for state estimation one needs to postulate the dy-
 356 namical model and only then implement techniques e.g. data assimilation or the ensemble
 357 Kalman filter techniques in order to estimate unknown variables and parameters in the
 358 model at all times and everywhere within the model domain. However, we demonstrate
 359 here that the machine learning framework is capable to estimate both ψ_1 and ψ_2 with a
 360 high average skill of about 0.7 (Figure 5). It is important to note that while ψ_2 is highly
 361 correlated with ψ_1 (average correlation coefficient is about 0.8) it is the decorrelated part,
 362 $\tilde{\psi}_2 = \psi_2 - A \psi_1$, that is dynamically important for the SSH evolution. The neural network
 363 is capable of skillful reconstruction of $\tilde{\psi}_2$ based on two SSH snapshots separated by 20 days,
 364 with an average skill of 0.7 for day 0 and a skill of 0.8 for day 20 (Figure 5). It is thus
 365 clear that mesoscale eddy patterns imprinted in SSH do provide substantial information on
 366 deep ocean currents or equivalently information on the partitioning between the baroclinic
 367 and barotropic modes even for baroclinically unstable flows. Nonetheless, since both lay-
 368 ers are dynamically active and no subsurface information is given by satellite observations,
 369 there is an inherent lack of information that is contained in sparse SSH observations and
 370 this prevents any interpolation or state estimation methodology from achieving a perfect
 371 skill. After all, if SSH snapshots are separated by a sufficiently long time, there should
 372 not be any relation between them due to the chaotic nature of ocean mesoscale turbulence.
 373 Nonetheless, we have demonstrated here that the 20 day separation even for a strong baro-
 374 clinically unstable current with a dynamically active subsurface flow does contain sufficient
 375 information for skillful interpolation and state estimation.

376 In providing a skillful state estimate from snapshots only, the deep neural network can
 377 essentially encode the underlying model equations and then utilize the information from
 378 subsequent SSH snapshot to even better constrain subsurface flows (see bottom panel in

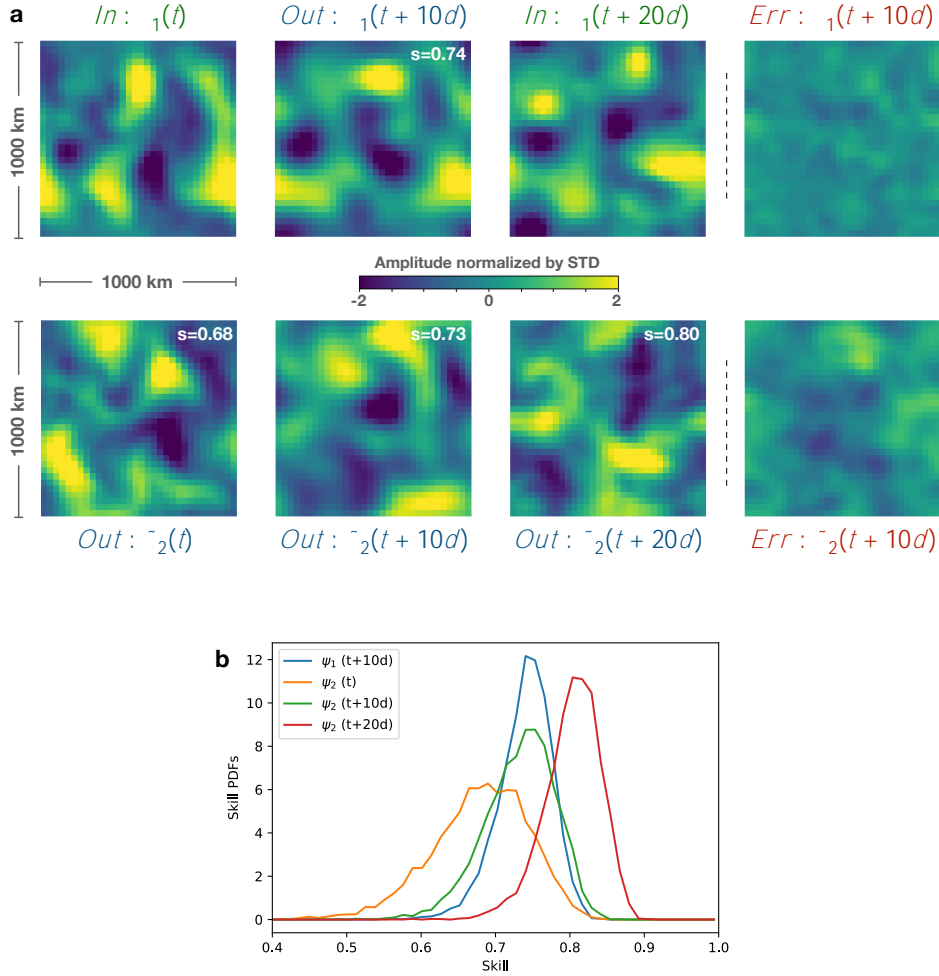


Figure 5. Examples of state estimation using Deep Learning neural network (a) and its statistical skill distribution for surface and subsurface variables at different times (b). As in the case of SSH interpolation, the neural network receives as input two SSH snapshots separated by 20 days, $\psi_1(t)$ and $\psi_1(t+20d)$ (top row, first and third columns), but reconstructs not only the surface streamfunction at the intermediate time, $\psi_1(t+10d)$ (top row, second column), but also the subsurface flow at all three times, $\psi_2(t; t+10d; t+20d)$. Note that ψ_1 and ψ_2 are linearly correlated with a correlation coefficient of 0.8, which is why the bottom rows in panel (a) show $\tilde{\psi}_2$, the component of the reconstructed deep flow that is not linearly correlated with the surface flow. The errors for reconstructing the day 10 surface and subsurface streamfunctions are shown in last columns. The probability density function of the neural network skill distribution is plotted in panel (b) for all predicted variables. Note, while the neural network provides skillful predictions for all variables (skill ranges from 0.65 to 0.85), the best prediction skill is achieved for subsurface flow at day 20 and the worst prediction is for subsurface flow at day 0.

379 Figure 5). It important to note the asymmetry in reconstructing subsurface velocities: at
 380 earlier times the skill is substantially worse (compare the orange and red curves in bottom
 381 panel of Figure 5). This asymmetry is expected in a chaotic and dissipative quasigeostrophic
 382 dynamics that makes it more difficult to estimate past state by observing the future as
 383 opposed to estimating future by observing the past. Thus, the two SSH snapshots must
 384 indeed be ordered in time as the PV-evolution equations only allow time reversal only for
 385 sufficiently small time intervals at which the dissipation effects can be neglected.

386 4 Discussion

387 Here we presented the proof of concept for using Deep Learning as an efficient tool to
 388 extract non-trivial information from sparse SSH observations, specifically demonstrating its
 389 utility in the spatiotemporal interpolation of SSH data and more generally in the state esti-
 390 mation that includes deep ocean currents apart from SSH. The Residual CNN outperformed
 391 the commonly used dynamical interpolation method. While it is challenging to precisely
 392 interpret the algorithm that was ultimately learned by the neural network, its success seems
 393 to be associated with its ability to predict subsurface flows only from individual snapshots of
 394 mesoscale eddy patterns. This separates machine learning from other methods that are in-
 395 capable of dis-entangling the highly-nonlinear relation between surface and subsurface flows
 396 and hence gives machine learning the edge in constructing a more accurate model of SSH
 397 evolution, resulting in higher quality interpolation.

398 Here we only considered the case of mesoscale turbulence and for the case of subme-
 399 soscale turbulence, the question remains open as to how SWOT’s 2D high-resolution swath
 400 measurements could be used to enhance the resolution of SSH data. While we expect the
 401 machine learning framework to perform well in reconstructing large and small mesoscale ed-
 402 dies, its limitations still need to be understood when considering mesoscale and submesoscale
 403 turbulence as a continuum. The main difficulty arises because the persistence timescale for
 404 submesoscale eddies is substantially shorter than for mesoscale eddies and no technique can
 405 bypass the inherent loss of the dependence on initial conditions for a chaotic system.

406 We have used a model of baroclinic turbulence as a synthetic training data because it
 407 presents a hard test for temporal SSH interpolation due to its chaotic nature and an a priori
 408 unknown impact of the dynamically active bottom layer on SSH evolution. We recognize
 409 that ocean regions where SSH variability is dominated by waves or other processes unrelated
 410 to baroclinic instabilities, a neural network that was trained to represent baroclinically
 411 unstable currents could perform poorly. Thus, it is necessary to develop more general
 412 training datasets that are more representative of the SSH dynamics for any given region of
 413 interest. Those could be ranging from more realistic mesoscale-resolving general circulation
 414 models to simplified stochastic QG-based models Samelson et al. (2019). Note, however,
 415 that it is essential for the synthetic model not to be overly simplistic to the point that
 416 it misrepresents the nature of SSH variability. The drawback of Deep Learning is that it
 417 generally requires a large number of data for training. Nonetheless, there are continuously
 418 improving methods aimed at addressing this practical issue, e.g. transfer learning (Pan &
 419 Yang, 2009) or one-shot learning (Fei-Fei et al., 2006).

420 A way towards ultimately developing the gridded SSH product using machine learning
 421 could be through training networks on a wide range of idealized and realistic models and
 422 then fine-tuning a much smaller number of neural network parameters using existing satellite
 423 data. However, since the true two-dimensional SSH state is not known at any particular time,
 424 the fine-tuning of a neural network cannot be achieved by defining a simple loss function as
 425 was done for synthetic data. Thus, the neural network ultimately would need to use a loss
 426 function that is based purely on observations, without invoking a dynamical model to provide
 427 a true state. This issue could be addressed for example using reinforcement learning, where
 428 two-dimensional SSH fields generated by the neural network would be rewarded or penalized
 429 based on the accuracy of their projection on the observed altimetry tracks that were left

430 out from the input set of tracks. Developing deep learning SSH interpolation techniques
 431 that would stir away from solely relying on dynamical models to provide training data
 432 is a necessary next step towards practical implementation with real satellite observations.
 433 Nonetheless, our work presents an important proof of concept, demonstrating that SSH
 434 observations do contain dynamically-relevant information about subsurface flows and hence
 435 with deep learning it is possible to build a skillful self-contained model of SSH evolution
 436 and as a consequence improve existing SSH estimates.

437 Finally we note another potentially important application of deep learning for state esti-
 438 mation at eddy-resolving scales. Since mesoscale-resolving data assimilation requires large
 439 computations, providing an accurate initial guess could substantially reduce the number of
 440 iterations necessary for optimization. It might be possible to accelerate data assimilation
 441 methods by providing the machine learning estimate as a first guess that is already close to
 442 reality. We thus see the synergy between machine learning and conventional state estima-
 443 tion methods as a potential framework for constructing improved state estimates, combining
 444 the best of the two paradigms: fast data-driven state estimation with machine learning and
 445 fine-tuning to ensure its strict consistency with a given dynamical model achieved by data
 446 assimilation.

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 453 flow/Keras along with the synthetic model datasets that were used in this study can be down-
 454 loaded here: https://drive.google.com/drive/folders/1tZrplLw2m19CB1YcQABj6pn0a7_-H63n?usp=sharing
 455

456 **References**

- 457 Abernathey, R. P., & Marshall, J. (2013). Global surface eddy diffusivities derived from
 458 satellite altimetry. *Journal of Geophysical Research: Oceans*, *118*(2), 901–916.
- 459 Aluie, H., Hecht, M., & Vallis, G. K. (2018). Mapping the energy cascade in the north
 460 atlantic ocean: The coarse-graining approach. *Journal of Physical Oceanography*, *48*(2),
 461 225–244.
- 462 Arbic, B. K., Scott, R. B., Flierl, G. R., Morten, A. J., Richman, J. G., & Shriver, J. F.
 463 (2012). Nonlinear cascades of surface oceanic geostrophic kinetic energy in the frequency
 464 domain. *Journal of Physical Oceanography*, *42*(9), 1577–1600.
- 465 Berloff, P. S., & Meacham, S. P. (1997). The dynamics of an equivalent-barotropic model
 466 of the wind-driven circulation. *Journal of marine research*, *55*(3), 407–451.
- 467 Bolton, T., & Zanna, L. (2019). Applications of deep learning to ocean data inference
 468 and subgrid parameterization. *Journal of Advances in Modeling Earth Systems*, *11*(1),
 469 376–399.
- 470 Carton, J. A., & Giese, B. S. (2008). A reanalysis of ocean climate using simple ocean data
 471 assimilation (soda). *Monthly Weather Review*, *136*(8), 2999–3017.
- 472 Chapman, C., & Charantonis, A. A. (2017). Reconstruction of subsurface velocities from
 473 satellite observations using iterative self-organizing maps. *IEEE Geoscience and Remote
 474 Sensing Letters*, *14*(5), 617–620.
- 475 Chelton, D. B., Schlax, M. G., & Samelson, R. M. (2011). Global observations of nonlinear
 476 mesoscale eddies. *Progress in Oceanography*, *91*(2), 167–216.
- 477 Davis, R. E. (1985). Objective mapping by least squares fitting. *Journal of Geophysical
 478 Research: Oceans*, *90*(C3), 4773–4777.
- 479 de La Lama, M. S., LaCasce, J. H., & Fuhr, H. K. (2016, 09). The vertical structure

- of ocean eddies. *Dynamics and Statistics of the Climate System*, 1(1). Retrieved from <https://doi.org/10.1093/climsys/dzw001> (dzw001) doi: 10.1093/climsys/dzw001
- 480
481
482 Ducet, N., Le Traon, P.-Y., & Reverdin, G. (2000). Global high-resolution mapping of
483 ocean circulation from topex/poseidon and ers-1 and-2. *Journal of Geophysical Research:*
484 *Oceans*, 105(C8), 19477–19498.
- 485 Fei-Fei, L., Fergus, R., & Perona, P. (2006). One-shot learning of object categories. *IEEE*
486 *transactions on pattern analysis and machine intelligence*, 28(4), 594–611.
- 487 Ferrari, R., & Wunsch, C. (2009). Ocean circulation kinetic energy: Reservoirs, sources,
488 and sinks. *Annual Review of Fluid Mechanics*, 41, 253–282.
- 489 Flierl, G. R. (1978). Models of vertical structure and the calibration of two-layer models.
490 *Dynamics of Atmospheres and Oceans*, 2(4), 341–381.
- 491 Fu, L.-L., Chelton, D. B., Le Traon, P.-Y., & Morrow, R. (2010). Eddy dynamics from
492 satellite altimetry. *Oceanography*, 23(4), 14–25.
- 493 Fu, L.-L., & Ubelmann, C. (2014). On the transition from profile altimeter to swath
494 altimeter for observing global ocean surface topography. *Journal of Atmospheric and*
495 *Oceanic Technology*, 31(2), 560–568.
- 496 Gaultier, L., Ubelmann, C., & Fu, L.-L. (2016). The challenge of using future swot data
497 for oceanic field reconstruction. *Journal of Atmospheric and Oceanic Technology*, 33(1),
498 119–126.
- 499 He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition.
500 In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp.
501 770–778).
- 502 Kingma, D. P., & Ba, J. (2014). Adam: A method for stochastic optimization. *arXiv*
503 *preprint arXiv:1412.6980*.
- 504 Klein, P., Isern-Fontanet, J., Lapeyre, G., Roulet, G., Danioux, E., Chapron, B., . . . Sasaki,
505 H. (2009). Diagnosis of vertical velocities in the upper ocean from high resolution sea
506 surface height. *Geophysical Research Letters*, 36(12).
- 507 Le Traon, P., Nadal, F., & Ducet, N. (1998). An improved mapping method of multisatellite
508 altimeter data. *Journal of atmospheric and oceanic technology*, 15(2), 522–534.
- 509 Pan, S. J., & Yang, Q. (2009). A survey on transfer learning. *IEEE Transactions on*
510 *knowledge and data engineering*, 22(10), 1345–1359.
- 511 Phillips, N. A. (1951). A simple three-dimensional model for the study of large-scale
512 extratropical flow patterns. *Journal of Meteorology*, 8(6), 381–394.
- 513 Samelson, R., Chelton, D., & Schlax, M. (2019). The ocean mesoscale regime of the
514 reduced-gravity quasi-geostrophic model. *Journal of Physical Oceanography*(2019).
- 515 Scott, R. B., & Arbic, B. K. (2007). Spectral energy fluxes in geostrophic turbulence:
516 Implications for ocean energetics. *Journal of physical oceanography*, 37(3), 673–688.
- 517 Smith, K. S., & Vallis, G. K. (2001). The scales and equilibration of midocean eddies:
518 Freely evolving flow. *Journal of Physical Oceanography*, 31(2), 554–571.
- 519 Targ, S., Almeida, D., & Lyman, K. (2016). Resnet in resnet: Generalizing residual archi-
520 tectures. *arXiv preprint arXiv:1603.08029*.
- 521 Ubelmann, C., Cornuelle, B., & Fu, L.-L. (2016). Dynamic mapping of along-track ocean al-
522 timetry: method and performance from observing system simulation experiments. *Journal*
523 *of Atmospheric and Oceanic Technology*, 33(8), 1691–1699.
- 524 Ubelmann, C., Klein, P., & Fu, L.-L. (2015). Dynamic interpolation of sea surface height
525 and potential applications for future high-resolution altimetry mapping. *Journal of At-*
526 *mospheric and Oceanic Technology*, 32(1), 177–184.
- 527 Vallis, G. K. (2017). *Atmospheric and oceanic uid dynamics*. Cambridge University Press.
- 528 Wunsch, C. (1997). The vertical partition of oceanic horizontal kinetic energy. *Journal of*
529 *Physical Oceanography*, 27(8), 1770–1794.
- 530 Wunsch, C. (2010). Toward a midlatitude ocean frequency–wavenumber spectral density
531 and trend determination. *Journal of Physical Oceanography*, 40(10), 2264–2281.