A new ocean dataset describing Boundary Current systems states and their variability

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Document History

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0.1	Sep. 1st, 2022	Guillaume Maze and Etienne Pauthenet	First draft to be discussed with partners (BSH, SOCIB, IPMA)
0.2	Sep. 10th, 2022	Ingrid M. Angel-Benavides and Estérine Evrad	Small edits and comments
0.3	Sep. 19th, 2022	All partners	Completed future plans in the last sections

EXECUTIVE SUMMARY

The task 2.3 of the WP2 EARISE package has an overarching goal to improve how Argo floats and data are used to study Ocean Boundary Currents (BC).

This deliverable is one component of the strategy toward this goal: using machine learning to improve Argo synergie with other observing systems in ocean state estimates. The other component of the task 2.3 strategy is to develop an Euro-Argo roadmap with regard to BCs (see D2.3).

Participants to task 2.3 identified boundary systems of interest:

- the Gulf Stream (IFREMER),
- the West Spitsbergen Current and East Greenland Current (BSH, IOPAN),
- the BCs in the Western Mediterranean region (SOCIB, SU)
- and the Gulf of Cadiz Current (IPMA)

First, we introduce why and how machine learning methods are useful to study BCs. These regions are intrinsically turbulent and chaotic dynamical systems. But machine learning methods thrive to identify relations between complex observations and to recognize hidden structures in multi-dimensional datasets such as Argo.

Second, we introduce 2 methods and a new monitoring dataset developed within WP2.3 for D2.8. The first method is completely new and at the edge of what's possible today with modern machine learning techniques. We combined neural network regression with ocean dynamics constraints in an artificial intelligence procedure to use complementary information from satellites and in situ ocean measurements. This method allows to produce a 3-dimensional time series with sufficient resolution to track meso-scale eddies at mid-latitudes. The second method is a specific application of an existing procedure called Profile Classification Modelling. This method uses unsupervised classification of Argo hydrographic profiles to identify the interior structure of the BC frontal regions. This method allows the production of a new descriptive dataset to monitor a BC system structure.

Last, we describe the way forward using the new methods in all BCs. Since the new methods have been developed using the Gulf Stream region as a test-case, we now have to apply them to all other BCs of interest. We present the procedure and software developed to do so.

TABLE OF CONTENT

1 Introduction

The ocean is a turbulent and chaotic dynamical system, therefore complex to understand and predict. This is particularly true in the western regions of the mid-latitude oceans, where very large currents narrow to intense fronts, meanders and numerous eddies about 100km wide. These regions are called "western boundary current extensions". Because they are turbulent, these regions are one of the main sources of uncertainty in the assessment of the ocean's role in climate and their behaviour under the influence of global climate change is still poorly known. These uncertainties can be reduced if we improve our ability to diagnose the temporal evolution of the three-dimensional structure of the extensions of the western boundary currents. More generally, these uncertainties arise in all turbulent regions and these are especially concentrated along Boundary Currents (BCs) that are at the centre of WP2 task 3. Figure 1 recalls all BCs of interest in WP2.3 but the reader is referred to the EARISE Deliverable D2.3 for a detailed rationale of boundary current systems and why it is important to observe them better.

None of the existing ocean observing systems is able to provide an accurate time series of three-dimensional eddy scale thermal fields for these boundary currents. Satellite measurements have a high local frequency and precise horizontal resolution, but they capture only the surface signature of the ocean's interior structures. On the other hand, in situ measurements of the interior of the ocean collected by autonomous probes such as Argo floats, provide a very accurate vertical thermal structure of the ocean, but they are rare and lack horizontal resolution.

Machine learning methods thrive to identify relations between complex observations and to recognize hidden structures in multi-dimensional datasets such as Argo (e.g. Bishop, 1995; Schmidhuber, 2015). In particular, (deep) neural networks are a non-linear regression method that has revealed itself to be very efficient to determine feature representation learned exclusively from data (Zhu, 2017). Therefore we proposed to develop a new product using a methodology based on neural network regression methods that have already been successfully tested in this context (Tokunaga and Maze, 2019; Agudelo, 2020). Neural networks are able to model complex and highly non-linear relationships between explanatory variables and therefore have the potential to appropriately capture the relationships between different satellite and ocean in-situ observations.

Among machine learning methods, those dedicated to clustering, i.e. unsupervised classification, are a perfect match for the task of identifying distinct vertical structures in BC regions (e.g. Bishop, 2006). Clustering tries to determine groups of samples with very similar features while being as much as different as possible to other groups of samples. Since a BC region is characterised by the presence of a front, i.e. a dynamical structure (mostly unstable) that separates at least two very different water masses, it is clearly tempting to use clustering to automatically identify these structures. However, this approach has only been started very recently (see Maze et al, 2017 for the method and Sambe and Suga 2022 for an application to the Kuroshio Extension BC region). We thus proposed to use clustering to better describe and monitor the state of the front and its associated water masses in BC regions of interest here.

2 Methodology

A. Non-linear regression with neural networks

We developed a new ocean prediction system called **OSnet** for “Ocean Stratification network”, which aimed at providing a physically consistent analysis of the upper ocean stratification in the Gulf Stream region (Pauthenet et al. 2022a). This system procedure is organised in 3 steps:

1. Assemble an **OSnet training set** where curated and interpolated in-situ profiles (mostly Argo but not only) are collocated with satellite data.
2. Fit an **OSnet predictor**: develop a neural network to learn from the training set how to predict temperature and salinity (T-S) profiles from space/time coordinates and satellite data. Also develop an adjustment method in order to correct and make predicted profiles physically consistent (no density inversions).
3. Predict an **OSnet 3D time series** on an easy-to-use regular space/time grid.

Assembling the **OSnet training set** is a laborious but quite straightforward procedure. We first download all the necessary dataset (CORA, Szekely et al, 2022, bathymetry, altimetry and sea surface temperature), then we extract a QC curated list of T/S profiles and interpolate them on standard pressure levels. Last, we collocate bathymetry, altimetry and sea surface temperature data values onto each curated profile. This dataset can be used for many purposes (pointwise study or development of any predictor).

For the **OSnet predictor**, the proposed scheme is a bootstrapped multilayer perceptron trained to simultaneously predict (i) temperature and salinity (T-S) profiles down to 1000m and (ii) the Mixed Layer Depth (MLD) from satellite data covering 1993 to 2019. The inputs are sea surface temperature and sea level anomaly, complemented with mean dynamic topography, bathymetry, longitude, latitude and the day of the year. The in-situ profiles are from the CORA database and include Argo floats and ship-based profiles. The prediction of the MLD is used to adjust a posteriori the vertical gradients of predicted T-S profiles, thus increasing the accuracy of the solution and removing vertical density inversions (Figure 2). The reader is referred to Pauthenet et al (2022a) for all the technical details.

The global normalised Root Mean Square Error (nRMSE) of T and S are better than a state-of-the-art ocean re-analysis (Glorys12) but worse than Armor3D[1] predictions (Figure 3). However, OSnet predictions do not have any unrealistic density inversions, while Armor3D does. Each OSnet profile is predicted independently, but OSnet produces coherent horizontal patterns on a 1/4◦ daily grid, especially for MLD. In addition, the pre-Argo years are well reconstructed, which supports the good generalisation skill of OSnet. The reconstructed surface temperature reproduces the observed warming trend. The seasonal cycle of surface salinity matches best the one of SSS (Sea Surface Salinity) compared to Glorys12 and Armor3D.

In Pauthenet et al (2022a) we made great use of the fact that the OSnet predictor can produce any type of ocean T/S/MLD fields (maps, timeseries, transects, etc…) in order to validate this new method. However, to make it easier for users to analyse OSnet predictions, we further developed **OSnet 3D time series** on a regular space/time grid. The method is straightforward, but again its application can be quite tedious, so we made predictions on our own regular space/time grid (the resulting dataset is about 660Gb) and published the result as an independent dataset. This is described further in the next section.

[1] Armor3D also combines in situ observations with satellite data to predict T/S profiles, but with a simple multi-linear regression (Guinehut et al, 2012).

B. Un-supervised classification

Maze et al (2017) introduced Profile Classification Modelling (PCM). A PCM allows the user to automatically assemble ocean profiles into clusters according to their vertical structure similarities. It provides an unsupervised, i.e. automatic, method to distinguish profiles from different dynamical regimes of the ocean. Figure 4 illustrates the PCM procedure: once the dimensionality has been reduced, profiles are clustered using a Gaussian Mixture Model. All technical details are provided in Maze et al (2017).

The PCM method has been applied to large basins like the North Atlantic (Maze et al, 2017; Desbruyere et al 2021), the Southern Ocean (Jones et al, 2019), the Indian Ocean (Rosso et al, 2020), and even the Amundsen Sea (Boehme et al, 2021). It has also been used to study frontal regions such as the Kuroshio Extension (Sambe et al, 2022) and the Southern Ocean (Thomas et al, 2021).

Here, the PCM procedure takes all historical in-situ Argo temperature/salinity profiles as input and produces a collection of the K most typical vertical profiles, or classes, as output (K is used-defined with possible recommendations from optimum statistical analysis). When applied to a boundary region, PCM thrives in identifying the typical vertical structures associated with each side of the front (because they are very different in shape, the classifier easily identifies them). Hence, within EARISE WP2.3 we have used PCM to characterise and monitor the Gulf Stream.

All notebooks used to conduct this analysis are available on the EA Collaborative framework at: https://github.com/euroargodev/boundary_currents_pcm/tree/main/docs/Gulf_Stream

Results are illustrated in Figure 5. It shows the typical vertical temperature profiles (5, 50 and 95% percentiles[2]) for the K=4 components, or classes, determined by the PCM to best describe the Gulf Stream frontal region. The K=0 class median profile (red curve) shows cold waters throughout the water column while the K=3 class profile is much warmer with a homogeneous warm layer down to 600m (the subtropical mode water) and a sharp decrease below. The K=1 and K=2 classes are intermediate profiles between the K=0 and K=3 extremes.

Figure 6 further shows the spatial distribution of profiles attributed to each of the 4 components. We can clearly see that the extremes K=0 and K=3 classes gather Argo profiles on the cold and warm flanks of the Gulf Stream, respectively. It is striking to see how a PCM, without any other information than the vertical thermohaline structure of the ocean, is able to automatically identify dynamically coherent regions in the ocean. We further observe that very few K=0 and K=3 profiles are found on the opposite side of the front (no K=0 in the south, no K=3 in the north). These are really the end tails of the thermohaline diversity in the region. On the other hand the K=1 and K=2 profiles are found all over the cold and warm flank of the Gulf Stream. These intermediate profiles are those found in meanders and eddies, precisely in areas of intense mixing.

3 New products and dataset

A. OSnet

The OSnet procedure described in the previous section leads to 3 main products that ultimately lead to a better characterisation of the Gulf Stream region structure and variability. In the next section we

[2] We take on all the profiles attributed to a given class and then compute the profile percentiles, e.g. 50% of the profiles are colder, 5% are colder, etc.

will describe how to extend the OSnet procedure to other BC regions. But let's now describe what these new products are about.

OSnet Gulf-Stream training dataset

As described before, we assembled a collection of curated and interpolated in-situ profiles (mostly Argo but not only, from CORA) collocated with ancillary data: bathymetry, mean dynamic topography, sea level anomalies and geostrophic current components from satellite altimetry, and sea surface temperature also from satellite. This resulted in the new "1993-2019 hydrographic profiles and colocated satellite data in the Gulf Stream" dataset (Pauthenet et al, 2022c) available here: https://doi.org/10.17882/89482

OSnet Gulf-Stream predictor

We also produced a python library to make T/S/MLD predictions in the Gulf Stream region using the Neural Network:

https://github.com/euroargodev/OSnet-GulfStream

Indeed, the whole procedure of the neural network prediction and mixed layer post-processing adjustment to suppress density inversions requires some expertise to be executed. Therefore, we developed a self-contained open-source Python library to make this easier to do. The library is packaged and distributed with the neural network and post-processing parameters. To make predictions with the OSnet Gulf-Stream predictor, users simply have to provide the space/time location they want T/S/MLD for. Users can also provide SLA/SST values for more accurate predictions, otherwise the library falls back on using climatological values for an approximate prediction. This software can thus be used to predict ocean transects, maps or Argo-like profiles in order to assess them in QC. This approach is much easier and light-weight, but as accurate, than downloading Gb of an ocean state estimate (eg, Glorys) and interpolating onto the user's needed space/time location. Using the OSnet predictor software is much easier and less storage intensive.

All these usage are demonstrated in this notebook:

https://nbviewer.org/github/euroargodev/OSnet-GulfStream/blob/main/docs/demo-predictions.ipynb

OSnet Gulf-Stream gridded dataset

As mentioned earlier, the OSnet predictor described in the previous section can be used to produce any type of ocean T/S/MLD fields (maps, timeseries, transects, etc…). To fulfil some users' requirements and make it easier to compare and assess OSnet predictions with regard to other ocean state estimates, we further produced a specific dataset where predictions were made on a 1/4 degree daily grid from 1993 to 2019.

This new dataset is called "Daily 3D maps of the T-S distribution in the Gulf Stream" (Pauthenet et al. 2022b) and available here: http://dx.doi.org/10.5281/zenodo.6011144

These four-dimensional fields of temperature and salinity, come with their associated confidence interval issued from the bootstrap. All the maps reveal coherent horizontal structures. At the surface, the warm Gulf Stream detaches from Cape Hatteras and meanders further east, transforming into the North Atlantic Current (Fig. 7a, b). The surface confidence intervals are maximum for the cold and fresh waters near the edge of the continental slope and inside the cold and fresh core eddies and meanders (Fig. 7c, d). At depth (1000m in Fig. 7e, f), the signature of large eddies is visible, associated with a maximum of the confidence interval again (Fig. 7g, h). The salty and warm Mediterranean Overflow Waters are seen in the southeast of the region. The average confidence interval at 1000 m is maximum along the Gulf Stream and its meanders, rather than in waters north of the Gulf Stream like at the surface.

B. BC monitor

Since all the codes developed for the PCM analysis are hosted on the EA-RISE collaborative framework at https://github.com/euroargodev/boundary_currents_pcm and written with the open-source language Python, we can further make use of the automation system offered by Github to monitor in near real-time all BCs, using index and figures produced throughout the PCM workflow.

Indeed, Github provides the "Actions" service, which allows automated workflows. Classically used for Continuous Integration, here it can be used to regularly run the PCM workflow and hence update profiles index file and figures. This can further be easily served on a webpage automatically updated with the last run of the workflow. This BC monitoring webpage is available here:

https://euroargodev.github.io/boundary_currents_pcm/

There are 2 main monitors that we now present.

1. Argo census

In order to classify profiles in BC regions, the first task is to actually create an index of the profiles located in such regions. This census is run automatically every 6 hours and uses the argopy software (also developed within the EARISE WP2 framework, Maze and Balem, 2020). Figure 8 shows how this census is presented on the BC monitor webpage. Badges with the number of profiles for each of the BC regions are displayed, and each badge links to a profile index file listing all profiles in the region (and obviously following the Argo profile index format). These badges can easily be inserted on any webpage of Jupyter notebook.

2. Supervised classification of profiles

Once profiles from a given BC region are listed, one can use a region-specific PCM to classify such profiles and report in near real-time on the interior structure of the BC region. At this point, only IFREMER has developed a PCM for the Gulf Stream. These pre-defined PCM are available here:

https://github.com/euroargodev/boundary_currents_pcm/tree/main/pcmbc/assets

We further provided an Argo like profile index with additional variables giving results from the PCM analysis (e.g. class labels).

All information is synthesised and given on the BC monitoring webpage, as illustrated Figure 9.

4 The way forward

IFREMER has been able to go through the process of developing a new dataset to characterise and monitor the Gulf Stream with machine learning techniques. IFREMER made all procedures and analysis (i) available online and (ii) flexible enough, in order to make it easy for partners to apply the procedures to their own BC regions of interest.

Extending OSnet to other BC regions

IFREMER assembled on the EA Collaborative framework a complete set of notebooks to go throughout the OSnet development procedure. These are located here:

https://github.com/euroargodev/OSnet/tree/extended

A complete documentation is also provided.

In spring 2022, a first extension of OSnet to the Nordic Seas was initiated by IFREMER in collaboration with BSH. Some examples of the preliminary results are given in Appendix B.

BC monitor for all regions of interest

This will require partners to develop a PCM for each of the BC regions of their interest. In order to do so, IFREMER has developed a tutorial notebook available here:

https://nbviewer.org/github/euroargodev/boundary_currents_pcm/blob/main/docs/PCM-demo.ipynb

IFREMER furthermore shared the specific notebooks used to develop the PCM for the Gulf Stream region (available here).

Once a PCM for each BC region will be settled on and made available online here, the BC monitoring webpage will be easily updated.

Plans until the end of the project

From now to the end of the project, IFREMER will continue to develop the documentation for the OSnet procedure and to provide support to partners for the extension of the BC monitor to other regions of interest. Beyond the EARISE project, IFREMER plans on extending the OSnet procedure to the global ocean and the BC monitor to all of the 5 subtropical gyre western boundary currents.

Until the end of the project BSH will develop a PCM method in both the West Spitsbergen Current and East Greenland Current based on the tutorial notebooks prepared by IFREMER to establish the BC monitoring in these regions.

In the future, a colaboration with other Euro-Argo partners with expertise in the Nordic Seas (IMR-Norway, IOPAN-Poland and DTU-Denmark) will be necessary to determine if the OSnet predictions are able to capture the water mass structures in the East Greenland Current. This boundary current has been chosen as a test-case scenario for the generalisation of the scripts and procedures developed for the Gulf Stream. However, there are important differences between both systems that could affect the OSnet prediction capacity. Specifically, the Nordic Seas has a considerably smaller Rossby radius (~ 1 km) and probably a weaker link between the surface signals and the vertical thermohaline structure. If the results in the East Greenland Current region are good, then the next step would be to use OSnet in the West Spitzbergen Current as well. The OSnet gridded T/S predictions would be useful for studying the transformation of water masses and the lateral heat fluxes in the Nordic Seas, for which eddies play a key role.

Before the end of the project, SOCIB will work to develop a PCM method for the Western Mediterranean Sea, which will include the Northern, Algerian and Balearic Currents. It will be based on the tutorials shown in this deliverable.

In regard to OSnet, in the future, SOCIB hopes to collaborate with IFREMER and Euro-Argo office to adapt these predictions to the BC located in the Western Mediterranean. Also, this task will be discussed with the expert SOCIB team to check if OSnet is able to capture the water mass structures associated to these interesting areas.

Until the end of the project, IPMA will follow the developments of the OSnet prediction system and the Profile Classification Method for the monitoring of the Boundary currents. The main goal is to use and implement these tools in the future, i.e. after the project.

5 Conclusion

We developed a new artificial intelligence procedure combining neural network regression with ocean physical constraints to produce a new dataset. This procedure has been applied with success to the Gulf Stream region and can be applied to any of the other BC regions considered here.

We also applied an existing machine learning technique to further describe BC systems with a classification method. This new dataset provides a complementary description of a BC region with regard to standard ocean state estimates. It has been applied to the Gulf Stream region and again could be applied to the other BC regions.

These new procedures and their associated software are all available online on the EA Collaborative platform.

Figures

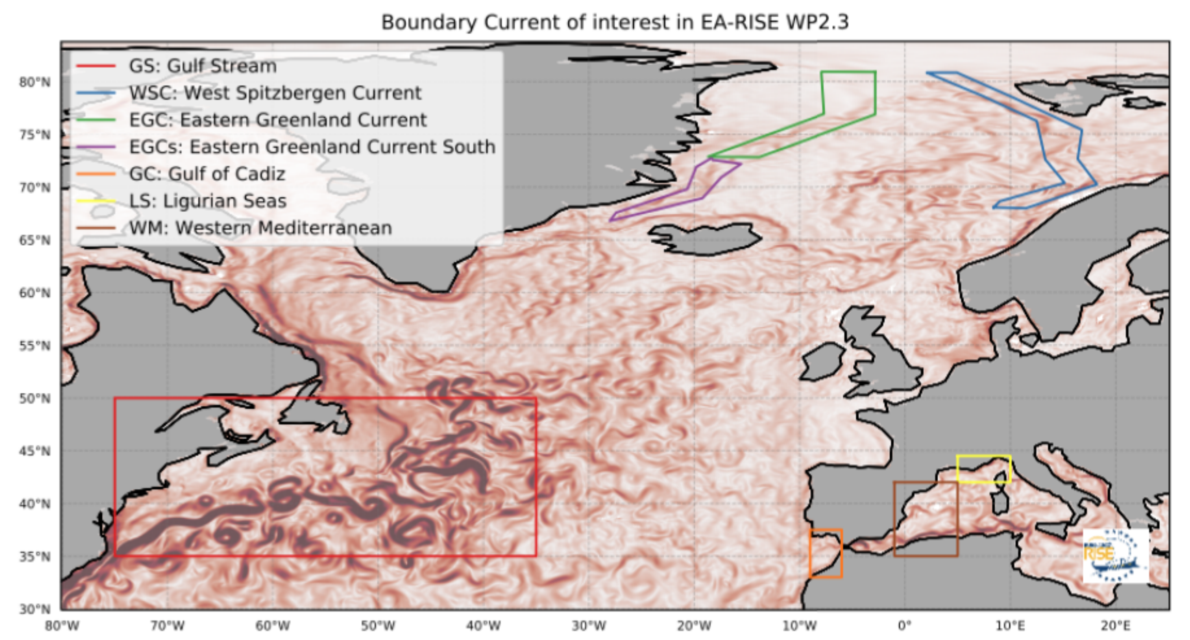


Figure 1. Synthetic map showing on top of the mean altimetry-derived currents all the Boundary Current systems of interest to Euro-Argo RISE WP2.3 partners.

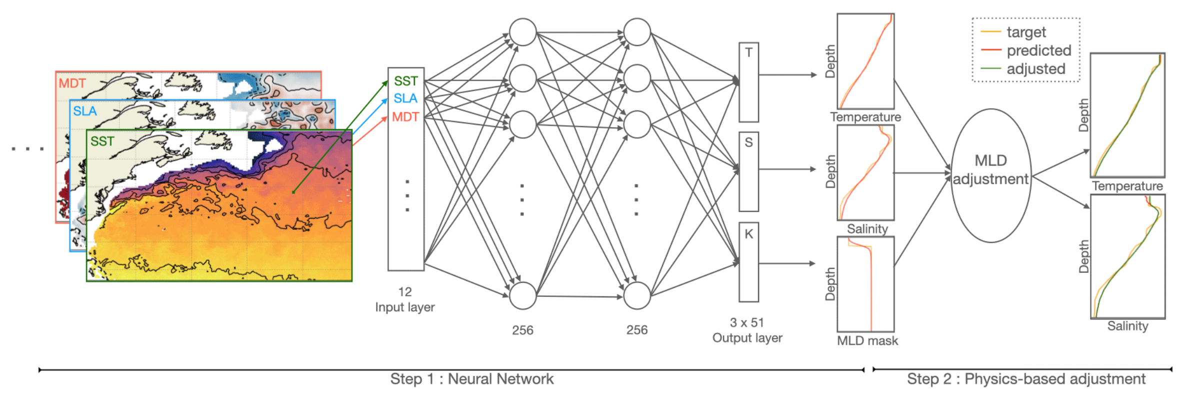


Figure 2. Schematic of the OSnet procedure formed of a neural network (NN) with two hidden layers and a mixed-layer (MLD) depth adjustment. The NN uses 12 surface inputs that are listed in Table 1 to predict profiles of temperature (T), salinity (S) and MLD mask (K). T − S profiles are then adjusted using the profile K for a better prediction of the MLD. Figure from Pauthenet et al (2022).

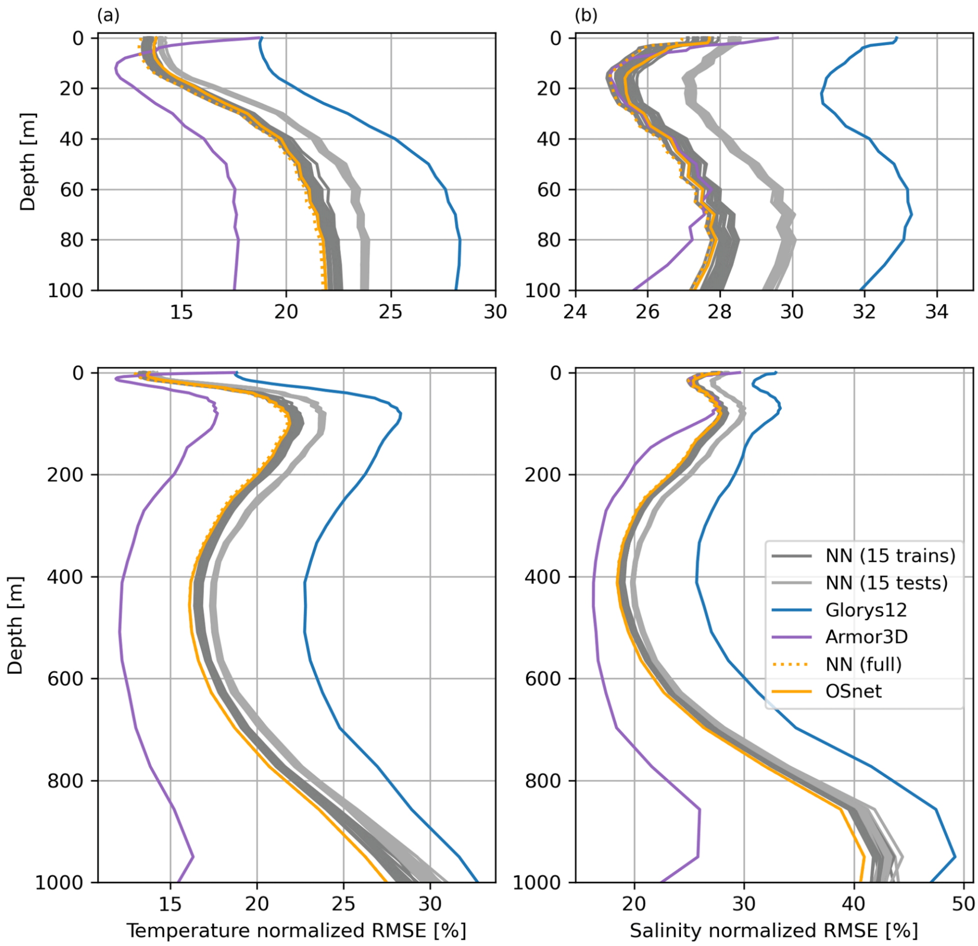


Figure 3. Normalised root mean square error (nRMSE) between temperature (a) and salinity (b) observed (CORA) and predicted profiles (Glorys12, Armor3D, Neural Network (NN) and OSnet). The normalisation is done with the standard deviation of the observed temperature and salinity by depth. The upper panels are a zoom of the first 100 m of the full-depth lower panels. The Glorys12 (blue) and Armor3D (purple) profiles are collocated with the CORA profiles, and the error is calculated between these subsamples. The NN profiles are only predicted with the NN, without adjustment of MLD, for 15 trained datasets (dark grey) and 15 test datasets (light grey). NN full (orange dotted) corresponds to the predictions using the full dataset (test + train) and is averaged for 15 models (bootstrap). Finally, the OSnet profiles (orange) are predicted with a NN bootstrapped 15 times and the MLD adjustment is performed, which slightly increases the error at the surface. Figure from Pauthenet et al (2022a).

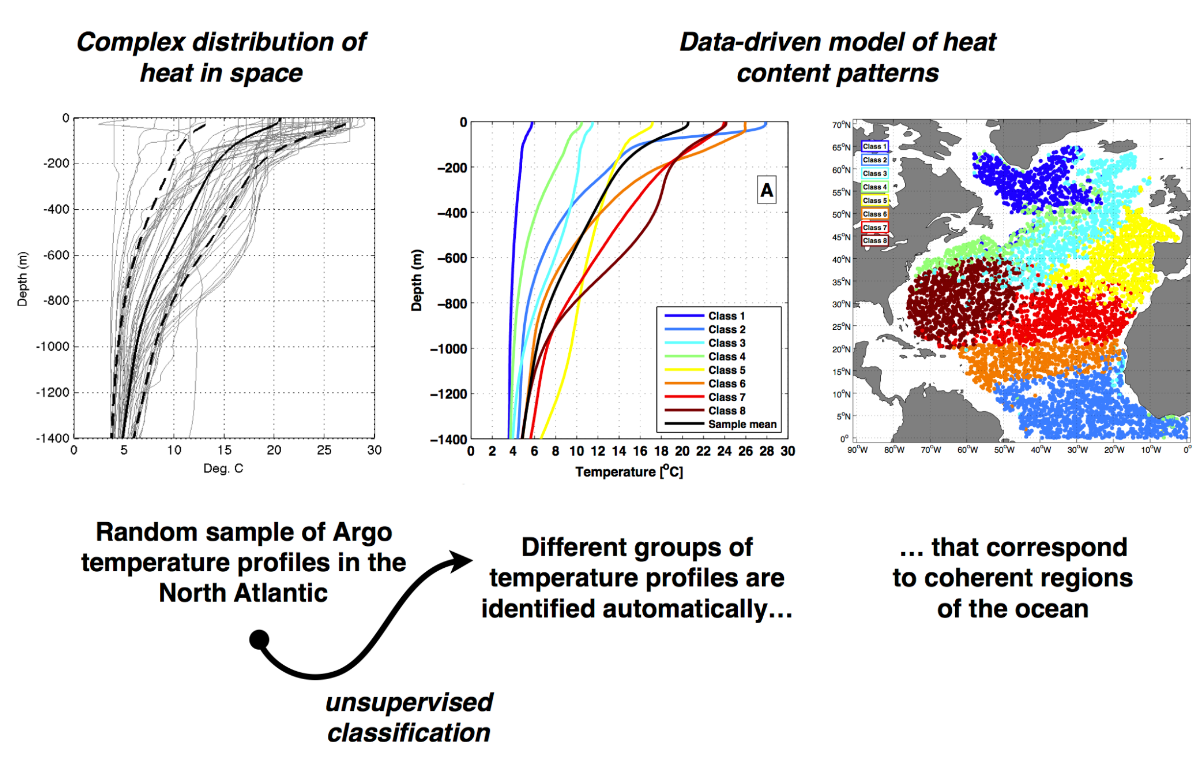


Figure 4. Simplified illustration of the PCM method. Here we use PCM to identify each side of a turbulent front in a BC region.

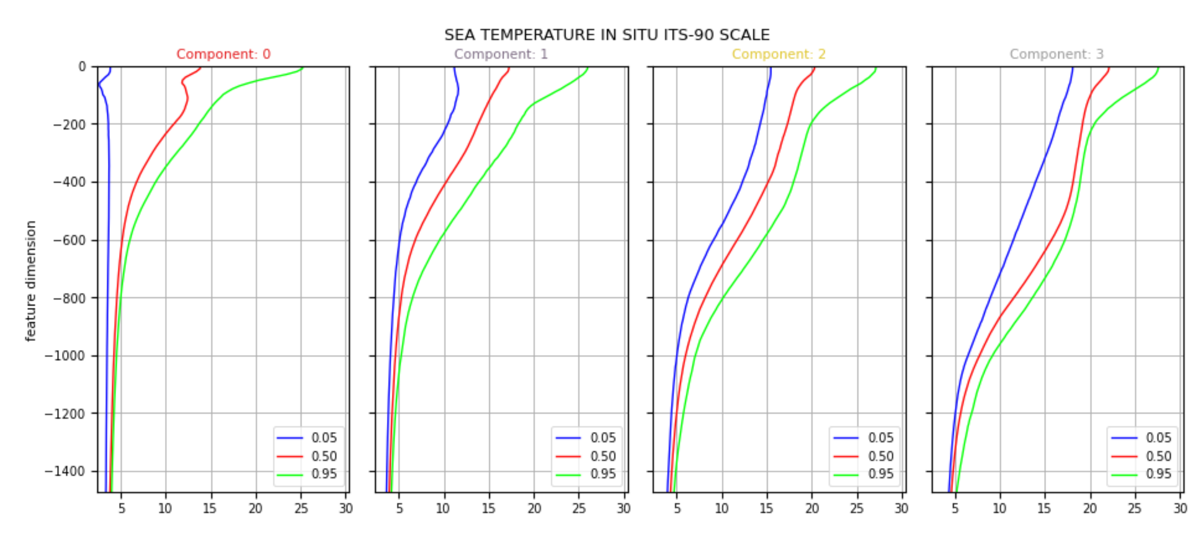


Figure 5. Typical vertical temperature profiles (5, 50 and 95% percentiles) for the 4 components, or classes of the Gulf Stream PCM.

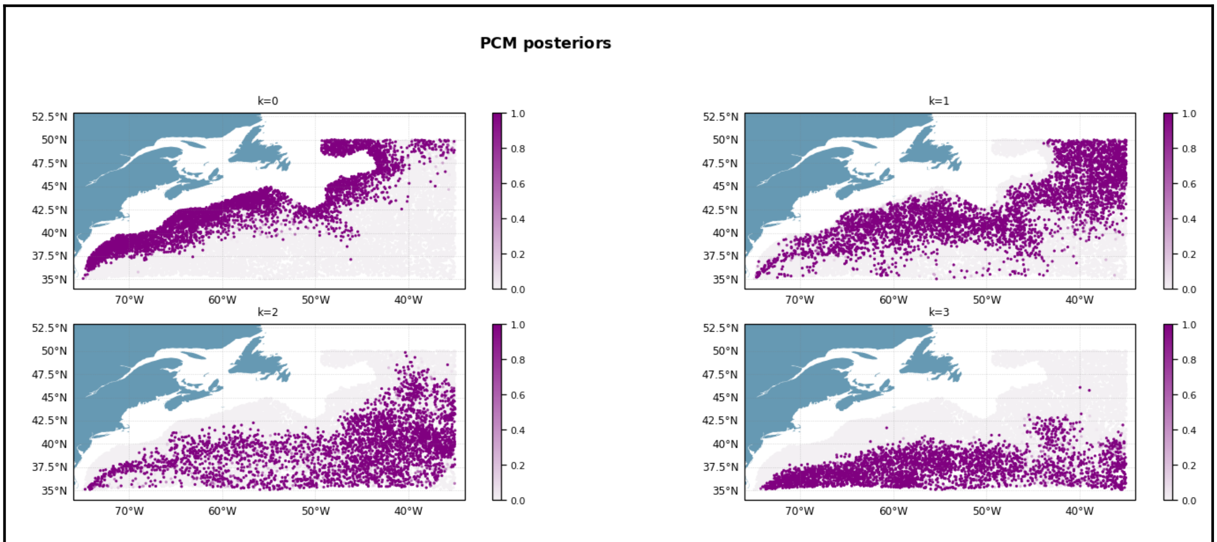


Figure 6. Probability (posteriors) of all Argo profiles to belong to each of the 4 clusters automatically determined to best describe the Gulf Stream region.

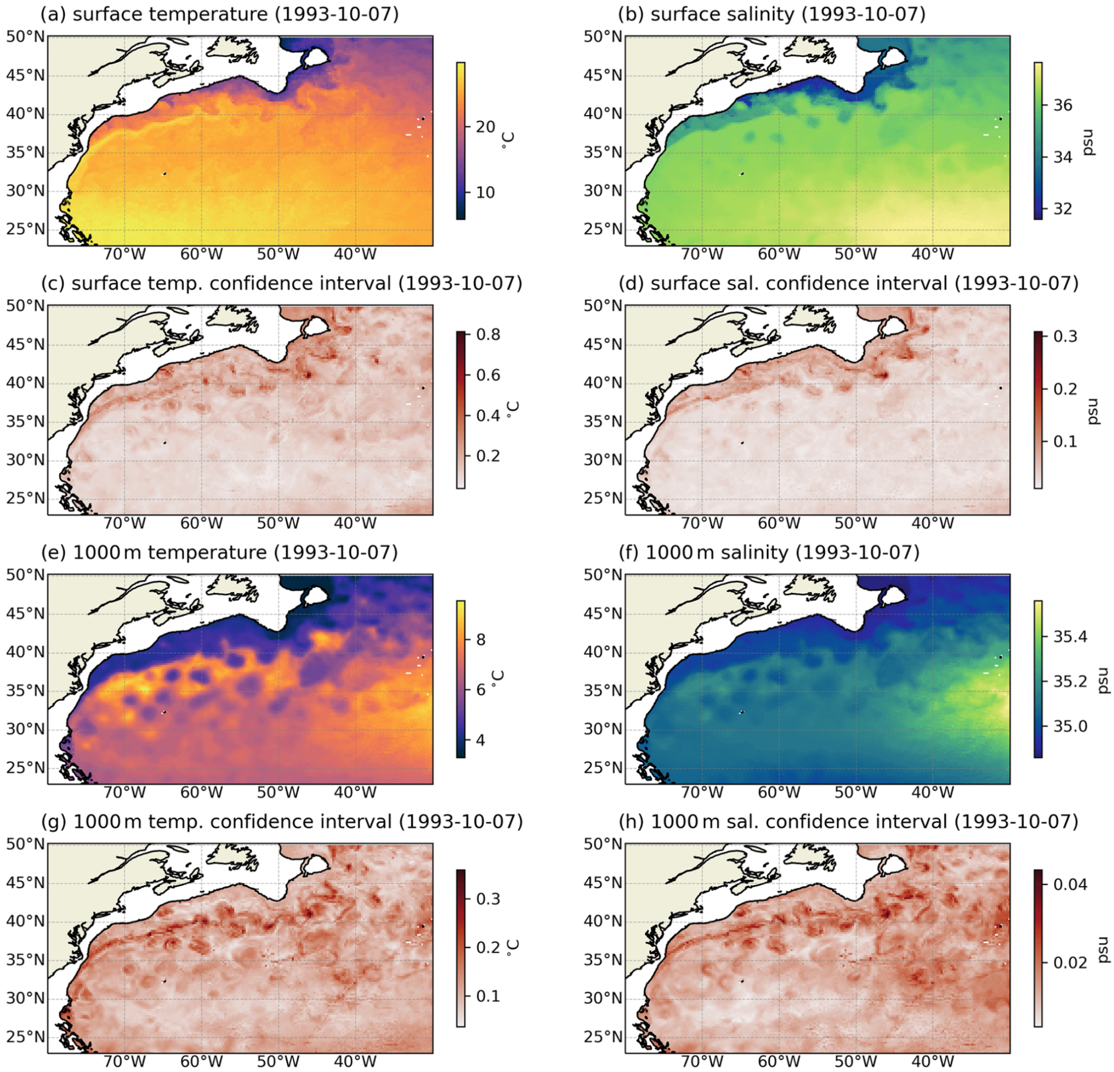


Figure 7. OSnet temperature and salinity maps for 7 January 1993, at the surface (a, b) and at 1000 m (e, f). Their respective confidence intervals are displayed too, i.e., the standard deviation of the 15 bootstrapped models (c, d, g, h). Figure from Pauthenet et al (2022b).

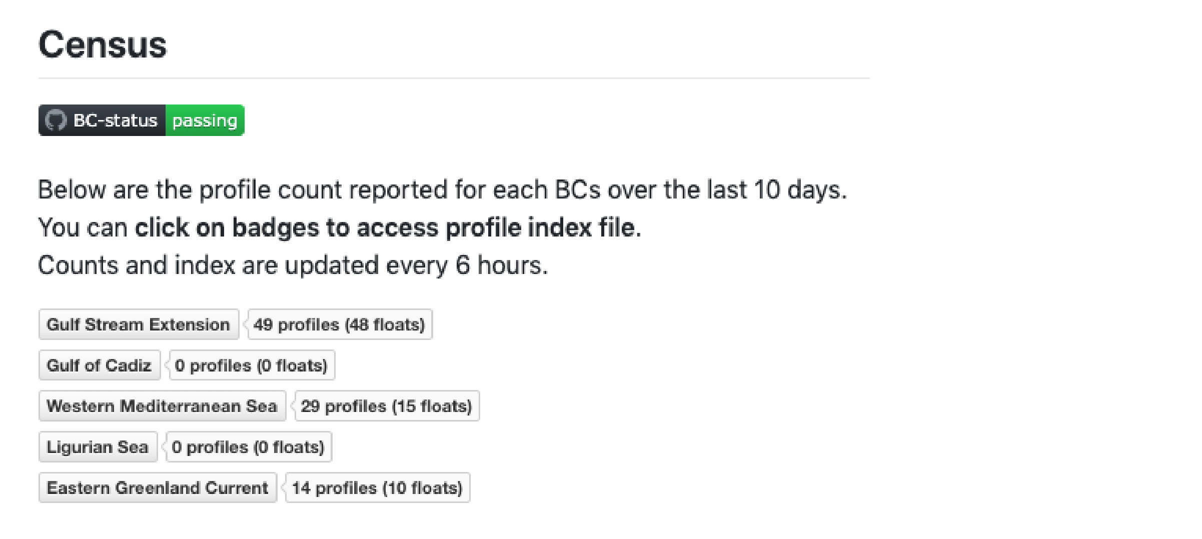


Figure 8. Screenshot of the BC monitor web page section with the near-real time Argo floats and profiles census in BC regions (access here).

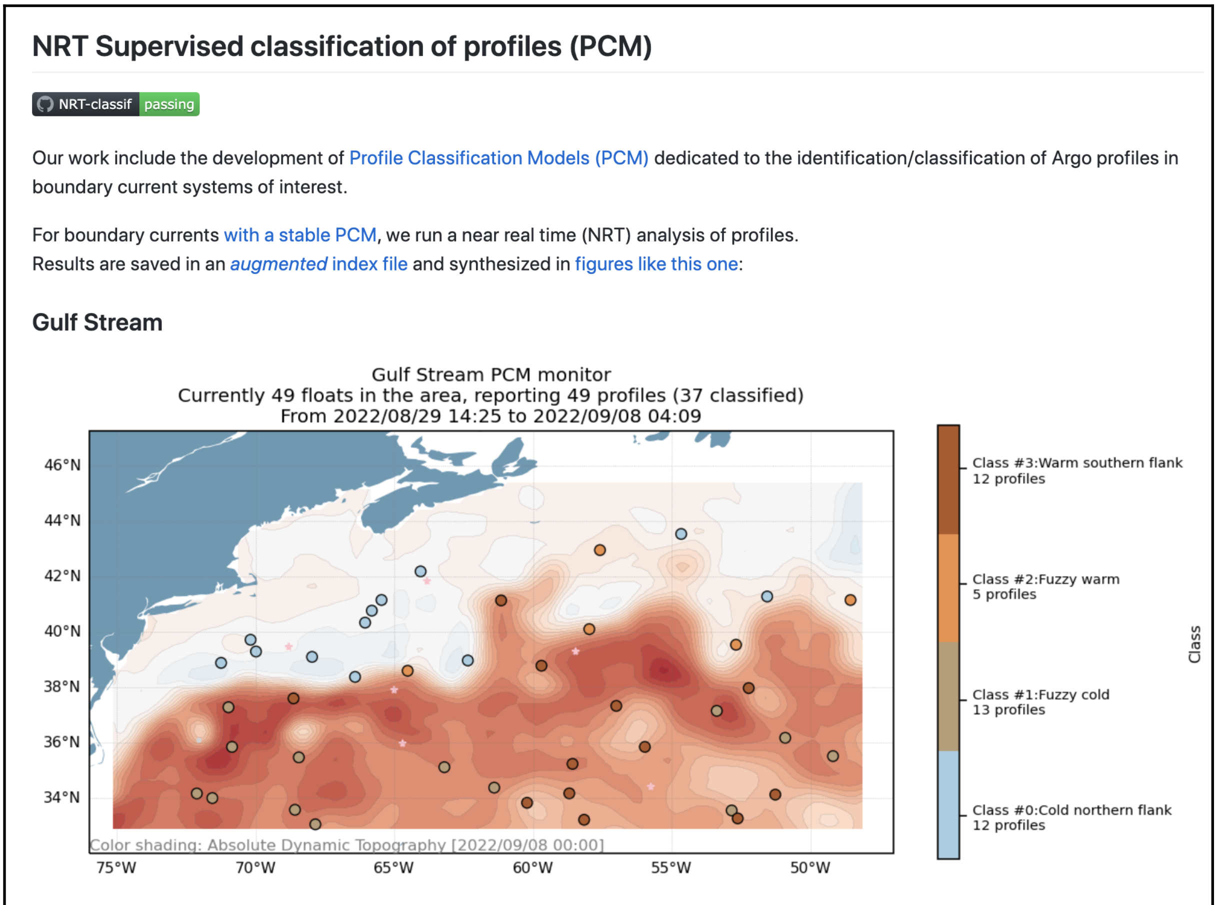


Figure 9. Screenshot of the BC monitor web page section with the near-real time Argo floats supervised classification of profiles in BC regions (access here). At this point (Sep. 2022), only the Gulf Stream region is available; PCM for the other BC regions are under development.

Appendix A: Recap of new products and dataset

Softwares and tools

- OSnet: Learning in-situ hydrographic profiles from satellite data using a neural network:
  - Osnet Gulf Stream Development codes
  - Software to train OSnet in the Gulf Stream
  - Software to make predictions in the Gulf Stream
  - OSnet development code to be apply the method in other BC regions
- Profile Classification Modelling (PCM) for boundary currents: perform and analyse PCM of Argo floats in specific BC systems

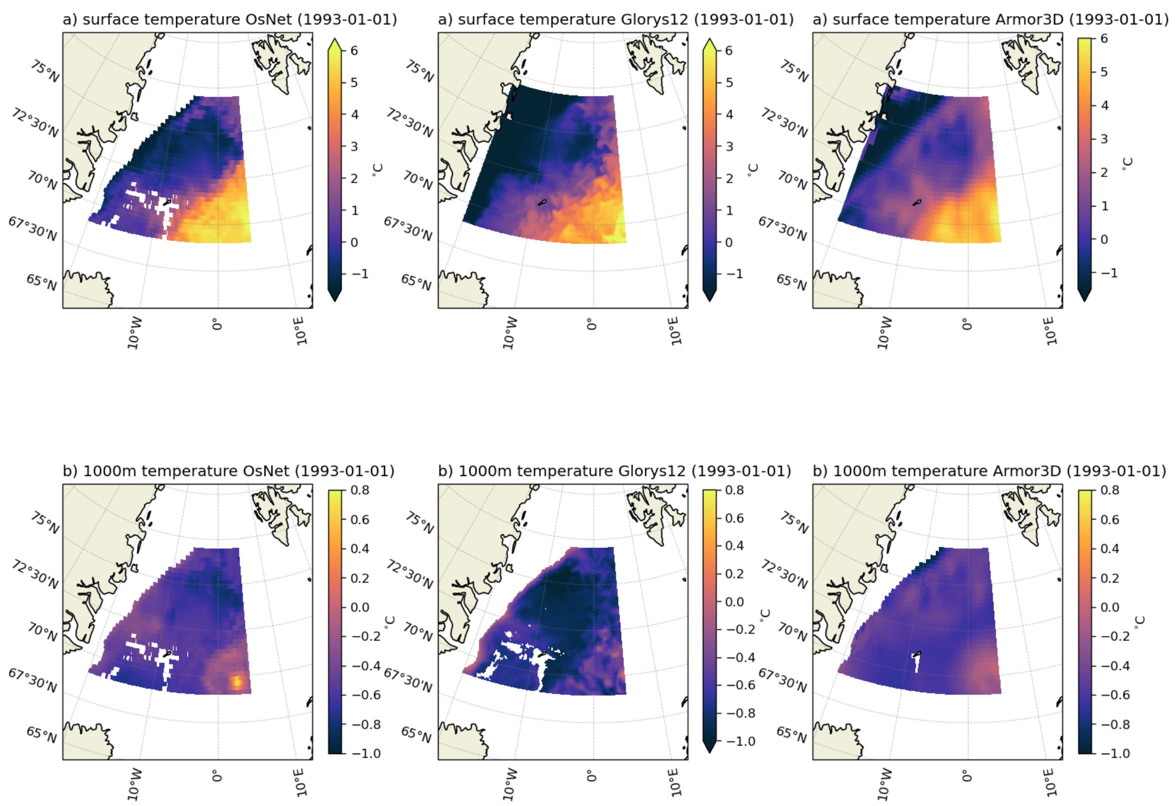
Products

- Pauthenet, Etienne, Bachelot, Loïc, Tréguier, Anne-Marie, Balem, Kevin, Maze, Guillaume, Roquet, Fabien, Fablet, Ronan, & Tandeo, Pierre. (2022). Gulf Stream Daily Temperature, Salinity and Mixed Layer Depth fields from Ocean Stratification network (OSnet). Zenodo. https://doi.org/10.5281/zenodo.6011144
- Pauthenet Etienne, Bachelot Loïc, Balem Kevin (2022). Training dataset for Ocean Stratification network (OSnet) in the Gulf Stream. SEANOE. https://doi.org/10.17882/89482

Appendix B: Extension to the Nordic Seas

In spring 2022, a first extension of OSnet to the Nordic Seas was initiated by IFREMER in collaboration with BSH. We succeeded in applying the OSnet workflow to this new region and to produce a daily time series of a 0.25x0.25 gridded dataset of temperature and salinity. This new product is still being investigated and validated, but the preliminary results are promising.

Figure below shows the OSnet-NordicSeas gridded dataset snapshot for Jan. 1st 1993 (as an example), at the surface and 1000m. For comparison, we also plotted the same fields from the GLORYS12 and ARMOR3D products. Once can see how realistic is the OSnet prediction, although no particular tuning or specific method adjustment have been performed yet.



Surface and 1000m depth temperature (top and bottom) for the OSnet, Glorys12 and ARMOR3D products, from left to right.

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