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Executive summary

This report presents steps for the design and implementation of a marine observatory providing current and forecasted oceanic conditions relevant to the aquaculture sector, with particular focus on “Extreme Marine Events”. Examples of successful implementation of these guidelines in the framework of the EuroSea project are presented for two aquaculture sites: Deenish Island in Ireland and El Campello in Spain. The process starts with stakeholder interaction to understand their main needs and concerns and is followed by the design of the software architecture that carries out the data acquisition, post-processing and visualisation in an open-access web platform. User feedback is of paramount importance during the whole process to ensure the services offered match the needs of the aquaculture sector.

Introduction

The ocean is of utmost importance to both the economy and the environment, acting as a regulator of climate shifts and supplying nations with food and resources (Bigg *et al.*, 2003; Lloyd and Vecchi, 2011; Winton *et al.*, 2013; Fleming *et al.*, 2019). Global climate change, greatly influenced by human activities and development, poses a major threat to the balance of highly sensitive areas like coastal marine systems, in which a large proportion of the population is located (Hoegh-Guldberg and Bruno, 2010; Abram *et al.*, 2019), and where a significant portion of the economy of these regions often relies on the aquaculture and fishing industries. These coastal areas possess immense social, economic, and ecological worth (Martínez *et al.*, 2007). Here, the potential production and exploitation of species of interest predominantly depends on the quality of the waters in which these activities are carried out. In this sense, fishing and aquaculture activities are greatly affected by changes of inherent oceanic variables, such as water temperature, hydrodynamics, pollution and non-native species (Hobday *et al.*, 2016; Brown *et al.*, 2019). For example, extreme events like marine heat waves (MHWs), characterised by periods of anomalously warm water temperatures that typically last for several weeks, can cause significant damage to marine ecosystems, and are becoming increasingly frequent and intense due to climate change (Frölicher and Laufkötter, 2018; Oliver *et al.*, 2018; Sen Gupta *et al.*, 2020). As a consequence, MHWs can cause detrimental effects to the environment, for example an increase in coral bleaching and, in the case of extreme events, mass mortalities of marine life. Increase of harmful algal bloom events are sometimes associated with such events with reports of persistent invasive species like the recent case of the macroalgal species, *Rugulopteryx okamurae* (Navarro-Barranco *et al.*, 2019; Faria *et al.*, 2022), which is expanding rapidly resulting in considerable economic and ecological impacts on the Atlantic and Mediterranean coasts of southern Spain and northern Morocco (Roca *et al.*, 2022).

In order to address extreme marine events and their socioeconomic impact, the need to develop and deploy robust oceanographic monitoring systems has become increasingly apparent in recent years. Stakeholders need to have easy and direct access to near real-time ocean observations of Essential Ocean Variables (EOVs) and ocean model forecasts of water conditions at global, regional and local scales. Ultimately, this enables the creation of sustainable development plans, both for marine industries and for the management of natural resources through the continuous analysis of near real-time and historical data (Tanhua *et al.*, 2019). In this sense, the European Commission contributes to the creation of projects that combine international collaboration of research institutions, universities and industry partners aimed at promoting the sustainable use of marine resources. For example, projects such as the Horizon 2020 project EuroSea focus on developing innovative technologies and methods for the monitoring, assessment, and management of marine resources across European waters, delivering ocean observations and forecasts to advance scientific knowledge and demonstrate the ocean's economic viability and importance to society in the long term.

Ocean observing can be achieved using a wide range of data collecting platforms. *In-situ* data, from oceanographic instruments, allows the monitoring of the ocean environment, the study of ocean circulation patterns, and the development of early warning systems (Soreide, Woody and Holt, 2001; Sendra *et al.*, 2015; Martínez-Osuna *et al.*, 2021). Oceanic numerical models allow the parametrization of the present and future behaviour of ocean variables (European Union-Copernicus Marine Service, 2016; Copernicus Marine Service, 2019). Remote sensing techniques, which include unmanned aerial vehicles (UAV) and satellite observations (Caballero *et al.*, 2022; Roca *et al.*, 2022), enable us to observe and measure a wide range of ocean variables such as Sea Surface Temperature (SST), ocean currents (sea surface height), and phytoplankton abundance (ocean colour). By integrating data information from the different ocean observing technologies described above, it is possible to create improved global ocean datasets and increase our understanding of the ocean environment.

In this study, we present the development of a multi-platform marine observing and early-warning system based on the interpretation of satellite, *in-situ* and modelled data. The platform provides access to the historical and real-time state of key physical, chemical, and biological ocean variables as defined by the Global Ocean Observing System (GOOS) and the Intergovernmental Oceanographic Commission (IOC) of UNESCO (Tanhua *et al.*, 2019). By providing ocean state information and future projections, we, together with our co-developers from the aquaculture industry, aimed to gain a better understanding of ocean dynamics to support sustainable fisheries management.

1. Ocean Application

1.1. Issue being addressed

Climate change is increasing the frequency, duration and intensity of so-called “Extreme Marine Events”, characterised by anomalous oceanic conditions over a sustained period that pose a threat to the health of marine ecosystems and organisms. Some examples of “Extreme Marine Events” include MHW and ocean deoxygenation.

Climate change will increase the pressure, not only on marine ecosystems, but also on marine economic activities, such as aquaculture. The impacts of climate change on the aquaculture sector can be summarised as follows:

- **Impacts on the health, growth and survival of the species of interest for the aquaculture sector.** Marine heat waves, characterised by anomalously high seawater temperatures for at least five days, cause significant stress to different aquaculture species, in particular to cold-water fish like salmon. Salmon (*Salmo salar*) is an important species in the aquaculture sector worldwide, and is cultivated on a large scale in Norway, Scotland, Ireland and the Faroe Islands. Elevated seawater temperatures reduce oxygen solubility and increase respiration rates. These effects, combined with high concentrations of organic matter derived from both phytoplankton blooms and the farming activity, can cause a severe impact on the dissolved oxygen concentration levels. Overall, the combination of high seawater temperature and low dissolved oxygen concentration increases the stress on cold-water fish species, with higher levels of stress making them more vulnerable to diseases and parasites such as sea lice.

- **In addition, climate change is expected to increase the frequency and severity of storms in some regions,** thus reducing the number of days with suitable working conditions to develop the necessary activities in an aquaculture farm. Severe storms can impact farm operations and damage critical infrastructure.

Therefore, in a global scenario of climate change, and with an increasing significance of aquaculture species as a food source, the availability of up-to-date information on current and forecasted oceanic conditions is of paramount importance for aquaculture activities. Having easy-to-access and accurate predictions of oceanic conditions and warnings on extreme marine events can help farmers take mitigation measures in advance. Furthermore, access to current and archived historical oceanic data can help them identify the reason behind issues in the aquaculture industry, such as a disease outbreak in the farm. This highlights the need for open-access portals where the oceanic information from different sources (*in-situ*, remote-sensing, models) can be easily obtained by the farmers, which is the objective of this best practice report.

1.2. Product of Best Practice

The product presented in this best practice report consists of guidelines or methodologies recommended for setting up a marine observatory where a monitoring station has been deployed and with focus on providing historical, current and forecasted oceanic conditions to the aquaculture sector.

1.3. Best Practice Description

1.3.1. Areas of study

Two monitoring stations have been deployed in aquaculture farms under the framework of the H2020 EuroSea project: Deenish Island in Ireland, and El Campello in Spain. These are the pilot sites where the methodologies and guidelines described in this best practice have been applied. The EuroSea project partner Xylem-Aanderaa was the manufacturer and developer of the sensors.

A. Deenish Island. The Deenish Island salmon farm is operated by Mowi Ireland and is located on the southwestern coast of Ireland at the mouth of Kenmare Bay. A monitoring station was deployed at 51.743°N 10.212°W in April 2022. The Atlantic Salmon (*Salmo salar*) is the most important species grown at the farm. Since salmon requires cold waters (< 17°C) for healthy growth and development, the main concern of farmers in this area is related to ocean warming and the expected increasing frequency of marine heat waves. The sensors in this buoy monitor winds, currents, temperature, salinity, pH, dissolved oxygen saturation and relative fluorescence. In order to provide a wider picture of the oceanographic conditions affecting the farm, remote-sensing data and particle-tracking predictions of the coastal circulation are also provided for an area spanning from 50.0 °N, 11.6 °W to 52.8 °N, 8.0 °W (Figure 1).

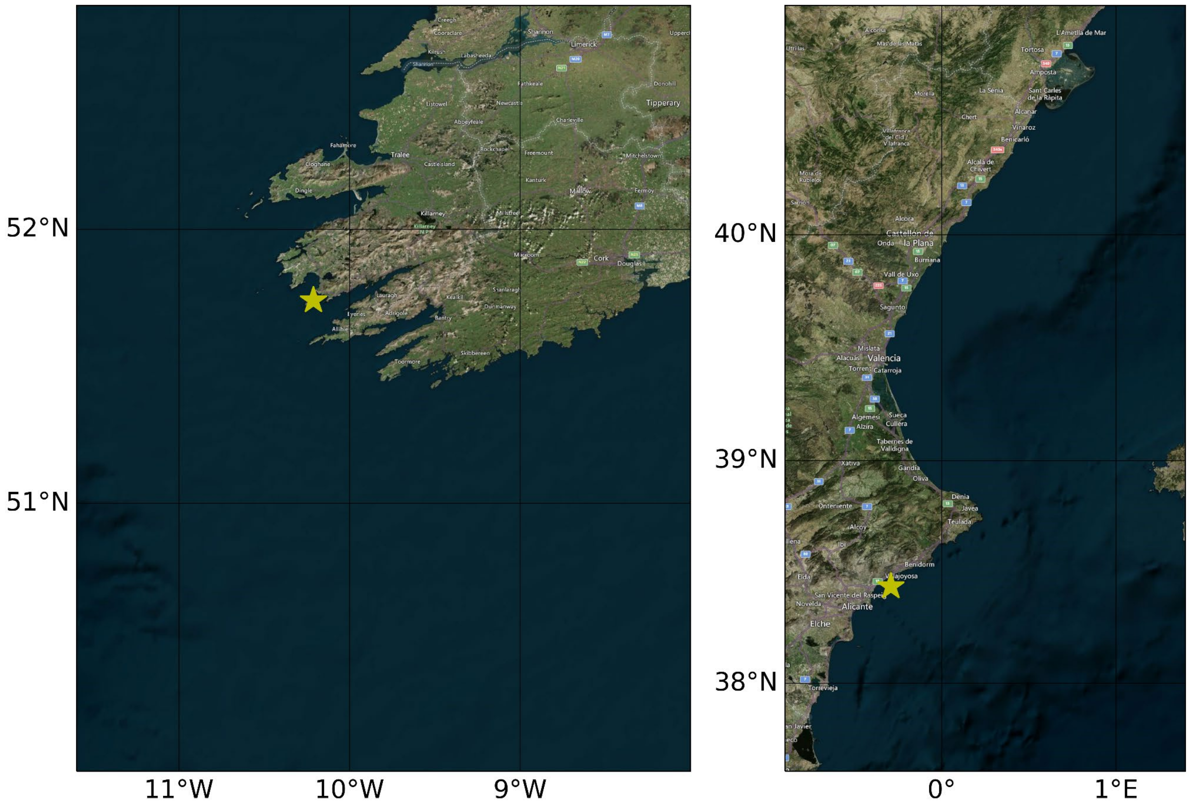


Figure. 1. Deenish Island site and wider area for remote-sensing data and particle-tracking predictions (left). El Campello site and wider area for remote-sensing data and particle-tracking predictions (right).

B. El Campello. The El Campello fish farm is operated by AVRAMAR and is located in the Mediterranean at 38.437°N 0.292°W, where a monitoring station was deployed in September 2022. Different fish species are grown at El Campello, including the European bass (*Dicentrarchus labrax*) and the gilt-head bream (*Sparus aurata*). The farmers are mostly interested in obtaining predictions and warnings of adverse weather conditions affecting the working operations at the farm. The sensors in this buoy monitor winds, waves, currents, temperature, salinity, turbidity, dissolved oxygen and relative fluorescence (chlorophyll). In order to provide information on a larger scale, remote-sensing data is provided for an area spanning from 37.6 °N, 0.9 °W to 41.0 °N, 1.4 °E (Figure 1).

1.3.2. Output type and description

The software architecture of the web portal follows a multi-container approach, where four different pre-processing containers communicate with the webapp container through a shared volume (Figure 2). These four pre-processing containers are responsible for downloading, processing, and formatting the data in a format that can be understood by the web application. The output data are then shared with the webapp through a shared volume. These processes are set to run periodically, so that the website is continuously updated with the new data.

A. Every ten minutes, the ***site*** container downloads the buoy data from an SFTP server hosted at enoc.puertos.es. It applies a quality control on the data and determines whether any marine warning (e.g., marine heat wave) should be set up based on the observational data.

B. The ***model*** container downloads model forecasts from the Copernicus Marine Service. It runs once a day.

C. The ***rs*** container runs once a day to download the remote sensing datasets.

D. The ***lptm*** container runs the particle-tracking model. It runs once a day.

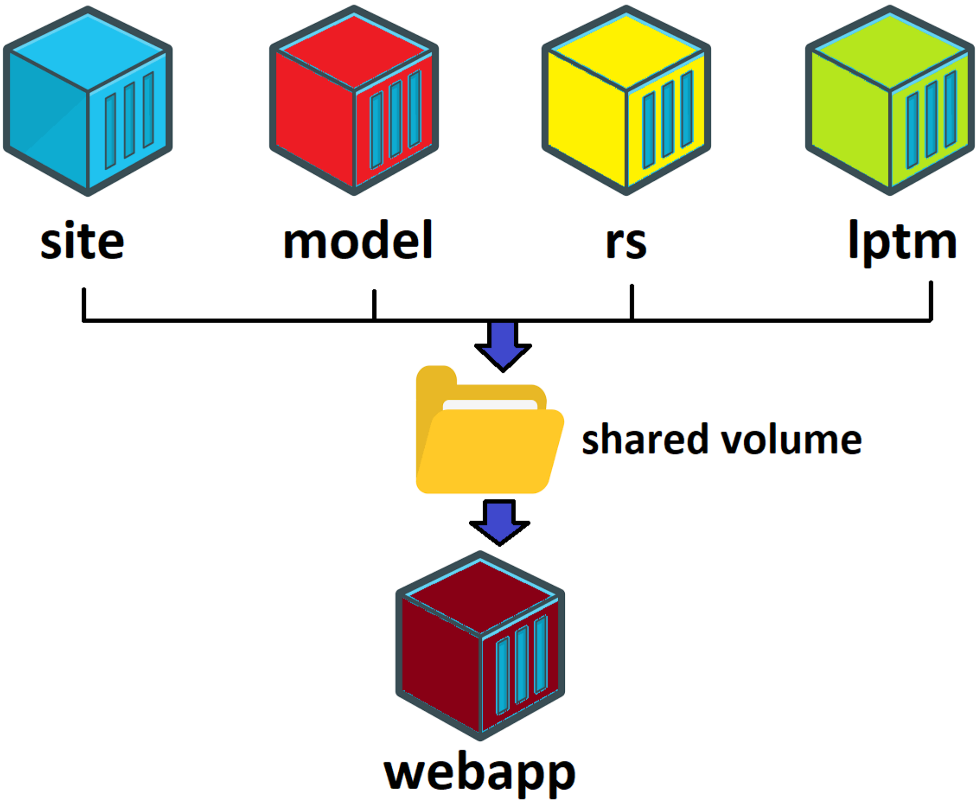


Figure 2. Scheme of the multi-container approach for deploying the website

All the output data are accessed and graphically represented by the ***webapp*** container whenever a user accesses the portal. The ***webapp*** container is also responsible for producing the output data files (CSV) for download, receiving user feedback and addressing the historical data requests. The subprocesses outlined in this section are expanded in detail in Section 1.3.2. below. Each of the pre-processing containers above (A-D) have to be duplicated for each separate application at different farming sites.

1.3.3. Steps for Implementation

Each of the sub-processes enumerated above are described in this section in detail, listing the different steps involved in a sequential manner, so that the guidelines described here can be replicated elsewhere.

1.3.3.1. In-situ data operations: the site container

The *in-situ* data operations consist of accessing and downloading the XML files delivered by the Xylem-Aanderaa instrument sensors; reading and storing locally the oceanic parameters of interest to the stakeholders, applying a quality control on the *in-situ* data, and sending the data to the shared volume so that it can be displayed on the website. This is described in the flowchart in Figure 3.

a. **Read configuration:** The *in-situ* operations are set to run every ten minutes, since this is the frequency at which new files are transmitted by the monitoring station. The first step involves reading a configuration file (CONFIG) containing the application-specific parameters. The CONFIG file is a text file with the following parameters defined: (1) *ndays*: the number of historical days that are displayed on the website as a time series graphics; (2) *SUR* (i.e. surface)*, MID* (i.e. middle)*, BOT* (i.e. bottom) Doppler Current Profiler cell indexes corresponding to the surface, mid-water and seabed measurements, the depth of which depend on local water column depth and the ADCP configuration; (3) *host* (e.g. Copernicus Marine Service *In Situ* TAC)*, user* (e.g. Copernicus user)*, pswd* (e.g. Copernicus password)*, folder* (e.g. folder inside Copernicus server which hosts the data from the buoy): these are the credentials needed to access the buoy data XML files in a remote SFTP (Secure File Transfer Protocol) server and the location of the XML data files within the server; (4) *clim_site*: a local file in the server that contains the SST climatological statistics (e.g. seasonal cycle and 90th percentile) for the geographical site of interest. The daily time series climatology for one year is displayed on the website and used to determine the occurrence of marine heat waves. The daily climatology is derived from a local, long-term SST record (e.g., from remote-sensing historical data) using the methodologies described in Hobday *et al.* (2016a).

b. **Get XML file list from local database:** The next step is to produce a list of the XML files already available in the local directory from previous executions. These files contain the recordings of different oceanic variables from the monitoring station sensors.

c. **Download new XML file:** The credentials (user, host, password) specified in the CONFIG file are used to establish an SFTP connection with the remote server where data from the buoy is stored in near real time. Any XML file located at the remote server that is not available locally is now downloaded.

d. **Load existing local dictionary:** The XML files contain a considerable amount of redundant information of no interest to the stakeholders. For this reason, some filtering is applied on the raw sensor data to separate out the irrelevant information (e.g., voltage, heading, tilt, acoustic ping count etc.) from the relevant oceanographic variables (e.g., temperature, salinity) needed for display on the website. This relevant information is organized as a data structure, or dictionary, and saved to a local file that is updated during every program execution (see “step g” below). This local dictionary is loaded into the memory. If it does not exist yet (e.g., first execution), an empty data structure is initialized.

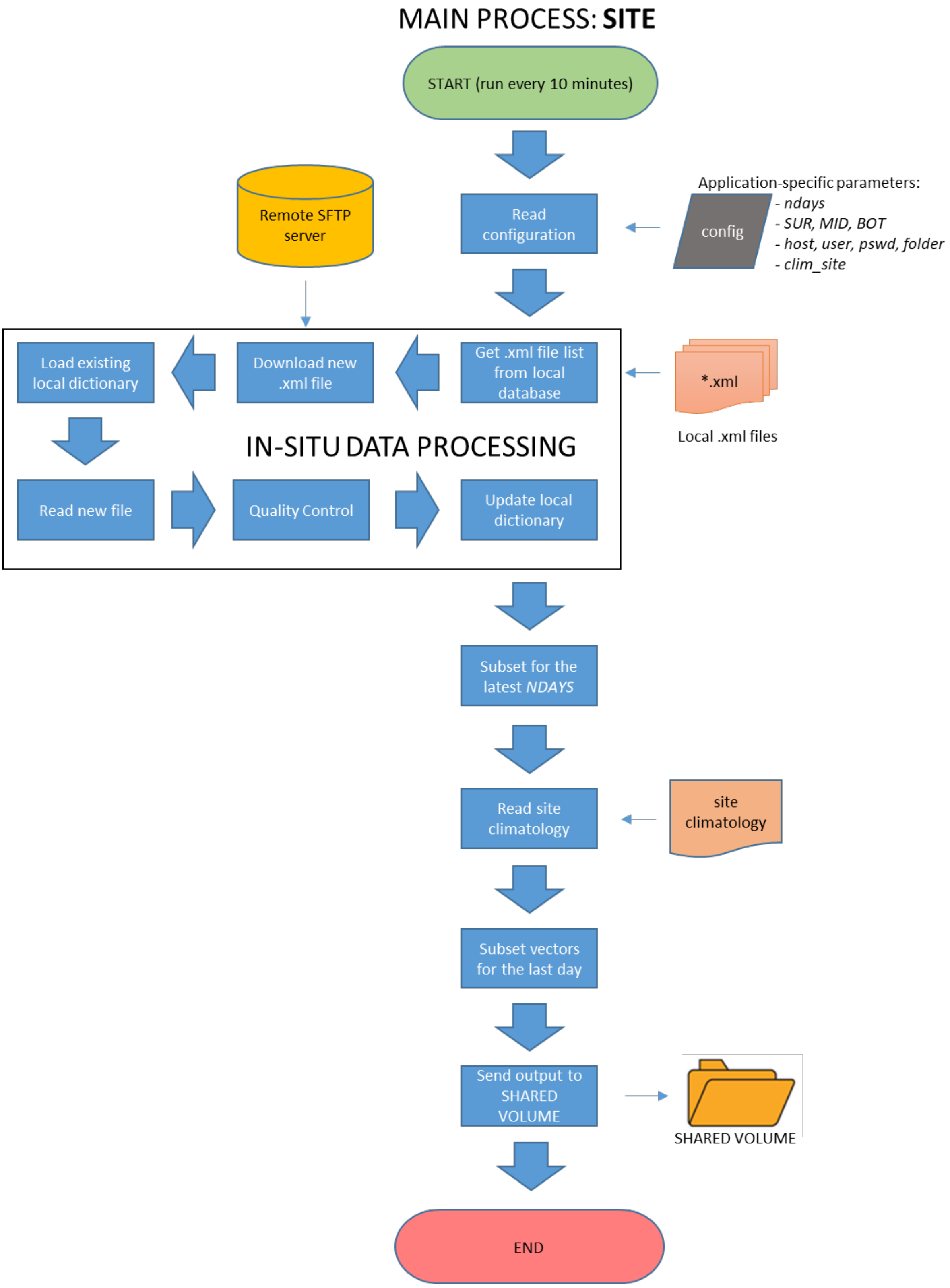


Figure 3. Flowchart describing the in-situ data operations

e. **Read new file:** The new file(s) downloaded in “step c” are read to retrieve the *in-situ* oceanographic buoy data. The ADCP cell indexes specified in the configuration file are used here to retrieve the appropriate oceanic current recordings at the surface, mid-water and seabed.

f. **Quality control:** A quality control of the raw input data is applied (see Section 1.3.7). It consists of flagging missing data and incorrect values (e.g., error code of the Deenish buoy while out of water was “68” for all sensors) with a “NaN” (*Not a Number*) value, and of ensuring that the time series has a constant time step of ten minutes from start to end. This means inserting “NaN” values when data are unavailable.

g. **Update local dictionary:** The local dictionary (data structure) loaded in “step d” above is now updated with the new data.

h. **Subset for the latest NDAYS:** All records from when the data buoy started to transmit data are handled by the historical portal application. While the historical data selection tool (see Section 1.3.3.5) facilitates the extraction of all available data, the Operational (Forecasting & Warnings) System, for better readability, only shows the most recent data. All visualisation decisions must be done in consultation with the stakeholders. The selected time period to show for all EOVs is specified in the CONFIG file (*ndays* parameter, see “step a”). In the case of directional data (e.g., winds, waves, and currents; see “step j” below) a short time period is recommended (e.g., 24 hours). For other EOVs, fourteen days were deemed sufficient (see Figure 4).

a. **Read site climatology:** The site climatology specified in the configuration file is read from a local file that must be produced for every application. This data is used to determine the occurrence of MHWs.

i. **Subset vectors for the last day:** In EuroSea, directional data (e.g., winds, waves, and currents) in the Operational (Forecasting & Warnings) System uses the last 24 hours of data. This is because directional data have a different graphical representation, not as a time series, but as a wind rose scatter plot (Figure 5). For the sake of clarity, only 24 hours are represented at 10-minute intervals on the portal to avoid an unclear, overcrowded scatter plot.

j. **Send output to SHARED VOLUME:** Warnings determined by the software and *in-situ* data gathered throughout the process is sent to the shared volume. All this information is accessible using the Operational (Forecasting & Warnings) System web application. Warnings refer to the occurrence of marine heat waves, wave heights of concern, and hypoxic conditions. Warning definitions are agreed with the stakeholders and will depend on their concerns (e.g., healthy environment for fish growth and development and/or safe working conditions at sea).

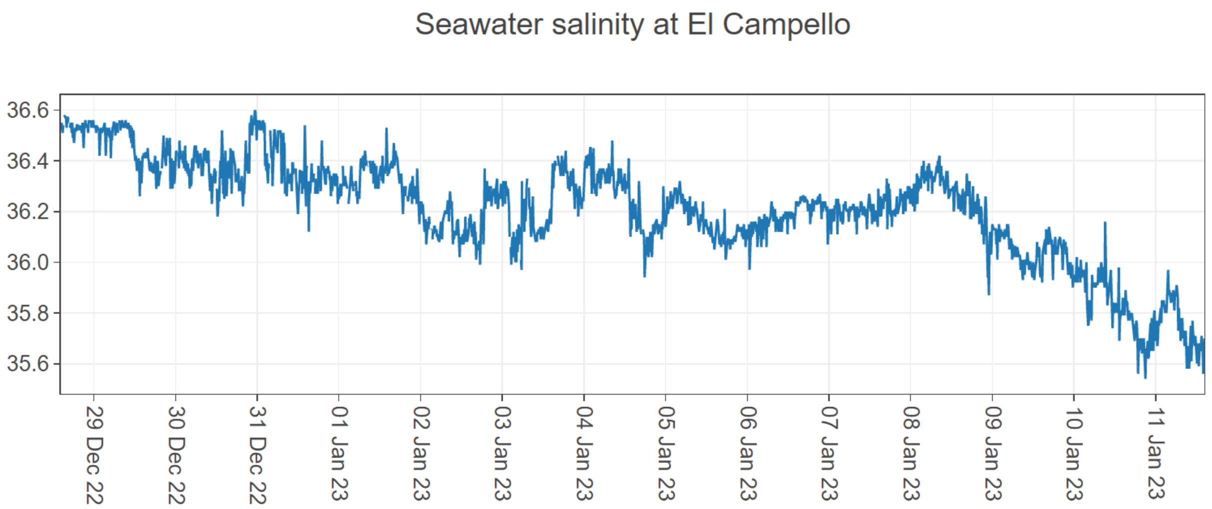


Figure 4. Time series showing two weeks of seawater salinity data at El Campello as displayed on the portal on 11-Jan-2023.

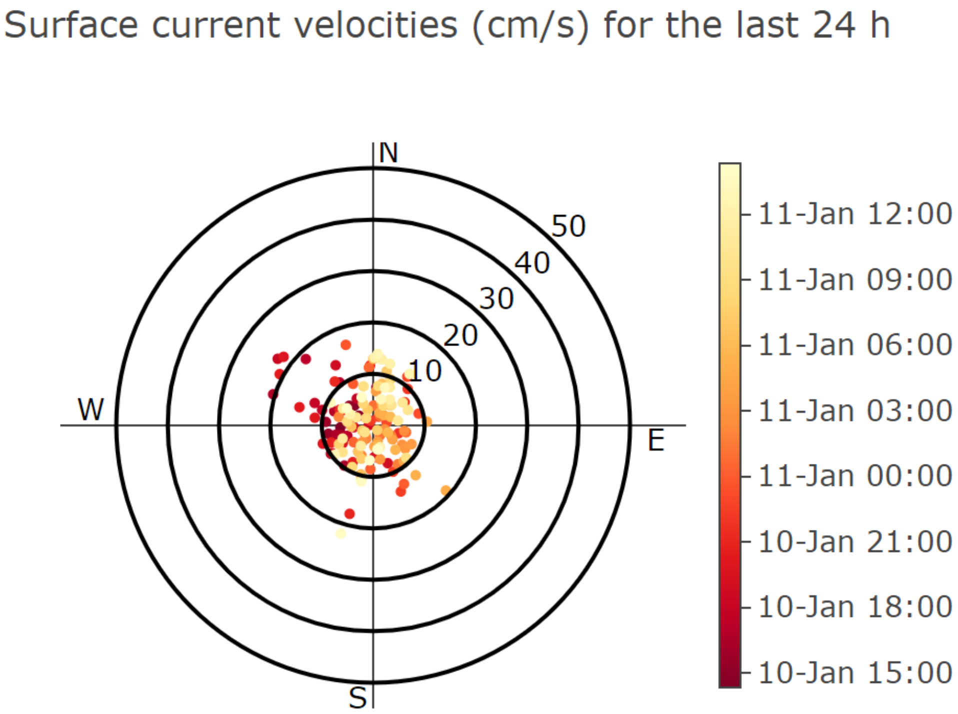


Figure 5. Wind rose scatter plot showing a 24-hour period of the surface current velocities at El Campello as displayed on the portal on 11-Jan-2023 at 14:30 hrs.

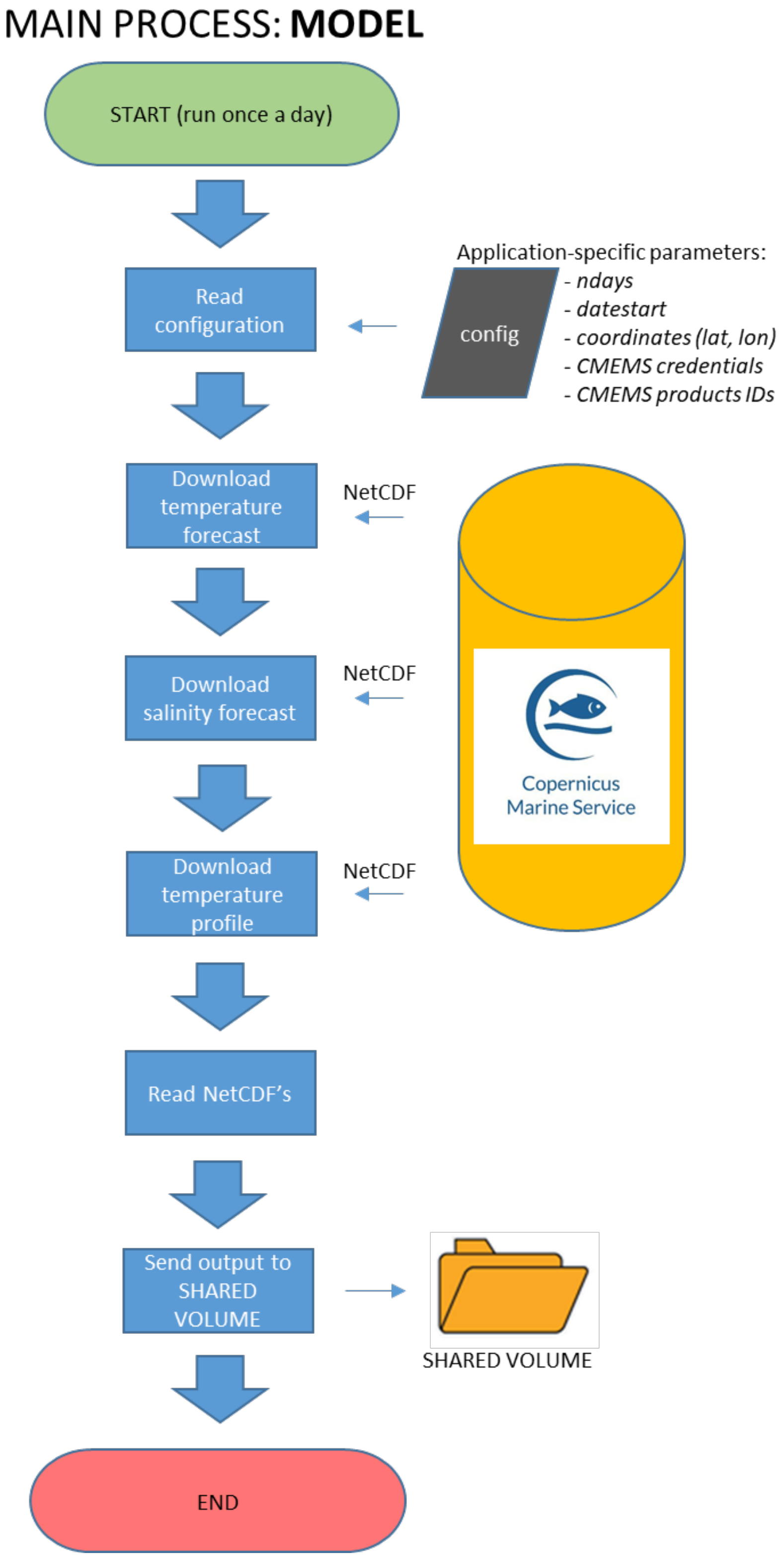
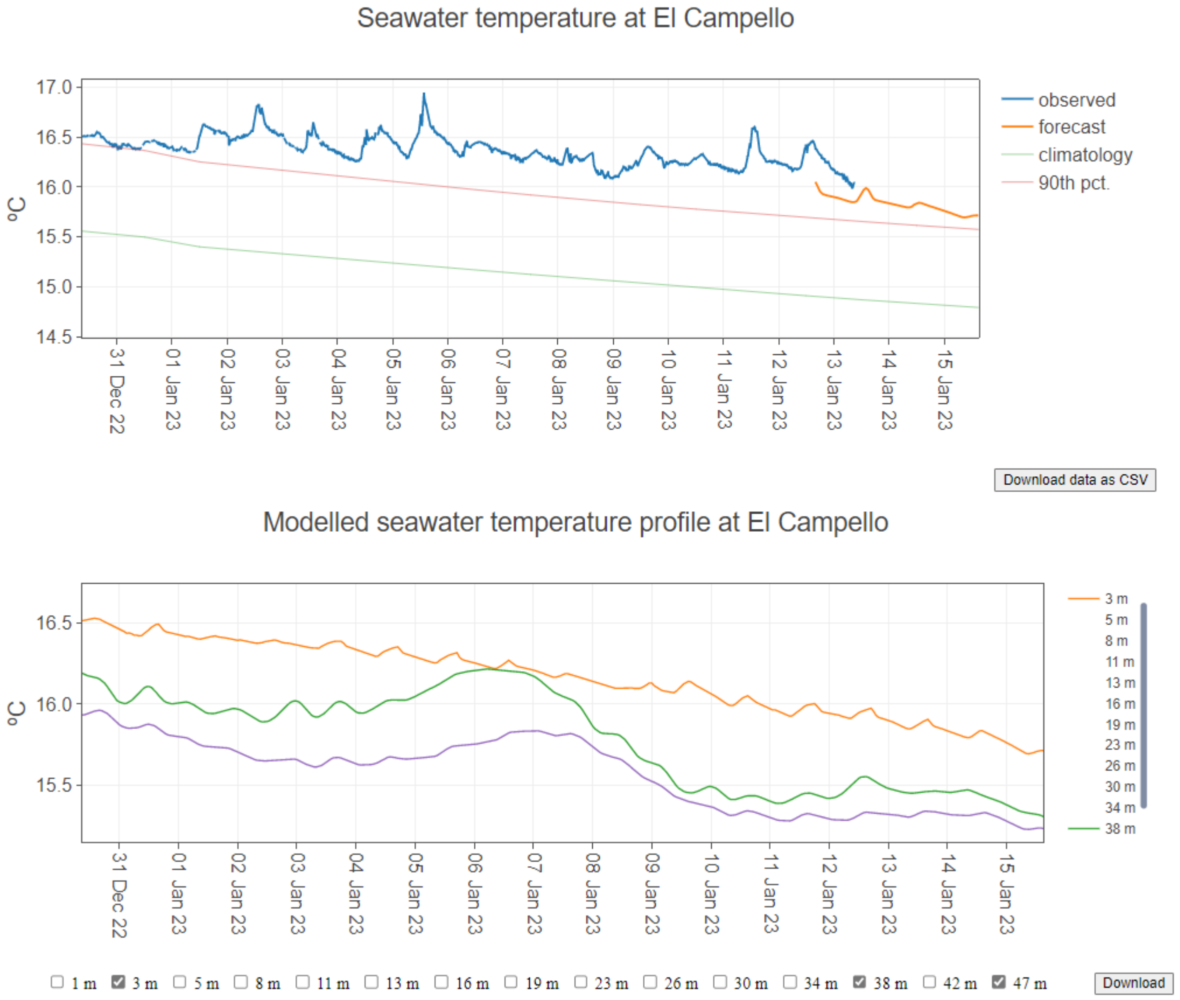


Figure 6. Flowchart describing the model data operations.

1.3.3.2. Forecasting and temperature profile data operations: the model container

The *model* operations basically consist of downloading the required datasets from the Copernicus Marine Service as NetCDF files, and then sending the data to the shared volume to be accessed by the web application (Figure 6). This process is set to run once a day. The required datasets are the forecasts (temperature and salinity) and the temperature profile. Stakeholders have shown interest in having information on the seawater temperature distribution throughout the water column and, since this is not provided by the sensors in the monitoring stations, the temperature profile is derived from hydrodynamic model products available in the Copernicus Marine Service.

Again, the first step is to read a configuration file, where different variables are defined, including: (1) the number of days back from today that will be displayed on the website for the seawater temperature profile, (2) the starting time to download a historical record of the seawater temperature profile, (3) the geographical coordinates of the mooring, (4) the Copernicus Marine Service username and password, and (5) the Copernicus Marine Service IDs of the desired products and services.



☐ 1 m ☑ 3 m ☐ 5 m ☐ 8 m ☐ 11 m ☐ 13 m ☐ 16 m ☐ 19 m ☐ 23 m ☐ 26 m ☐ 30 m ☐ 34 m ☑ 38 m ☐ 42 m ☑ 47 m

Figure 7. (TOP) In-situ temperature as recorded by the EuroSea monitoring station at El Campello (blue), together with the temperature forecast from the Mediterranean Sea Physics Analysis and Forecast service (orange), and the SST climatology for this site derived from the Multiscale Ultra-High Resolution (MUR) SST product. The mean seasonal cycle (green) and 90th percentile (red) are shown. (BOTTOM) Temperature profile from the Mediterranean Sea Physics Analysis and Forecast service. The user can select multiple vertical levels. Here, the 3-meter (orange) 38-meter (green) and 47-meter (violet) depth layers are shown. This is useful to examine the magnitude and variability of the thermal stratification over time.

For Deenish Island, the Atlantic - European Northwest Shelf - Ocean Physics Analysis and Forecast service (DOI:10.48670/moi-00054) is used. This service is a 1.5-km horizontal resolution NEMO application, forced by the ECMWF Numerical Weather Prediction model and assimilating SST, water temperature and salinity profiles and remote-sensing sea level anomaly data. The service provides 6-day forecasts, thus making it suitable for predicting the occurrence of marine heat waves in advance.

For El Campello, the Mediterranean Sea Physics Analysis and Forecast service (DOI:10.25423/CMCC/MEDSEA_ANALYSISFORECAST_PHY_006_013_EAS7) is used, a NEMO-based coupled hydrodynamic-wave model in a 1/24° horizontal resolution grid, with data assimilation of temperature and salinity profiles and remote-sensing sea level anomaly data. The service provides 3-day forecasts (Figure 7).

Surface temperature and salinity forecasts, together with seawater temperature profiles, are downloaded daily from the Copernicus Marine Service using the python-motuclient. Data are downloaded, in NetCDF format, only for the nearest node to the mooring deployment. Finally, the data are read and sent as a data structure, or dictionary, to the shared volume, where they can be accessed by the web application.

1.3.3.3. Remote-sensing data operations: the rs container

The *remote-sensing* operations: (1) download the latest SST map for the area of interest, (2) using an SST climatology, calculate the SST anomaly and analyse the occurrence of marine heat waves, (3) download the chlorophyll-*a* distribution from ocean colour observations, (4) determine the chlorophyll-*a* anomaly, (5) send the data to the shared volume to be accessed by the web application (Figure 8). Remote-sensing products complement the *in-situ* measurements by providing a wider picture of the surface temperature and chlorophyll-*a* distribution. This is interesting for the aquaculture sector to anticipate the occurrence of Extreme Marine Events at the farm, such as marine heat waves or harmful algal blooms.

In a similar way to the processes described above, the remote-sensing operations start with the configuration options, where the geographical boundaries (West, East, South, North) of the area of interest are entered. Moreover, the mooring coordinates, Copernicus Marine Service credentials and IDs of the desired products and services also need to be specified. Additional input files are required and have to be prepared before the process runs for the first time. These are a coastline file and an SST climatology file. The coastline, used later to render the maps on the website, can be derived from the GSHHG (Global Self-consistent, Hierarchical, High-resolution Geography) database (Wessel and Smith, 1996), which provides a worldwide coverage of the global coastlines at five different resolutions. The SST climatology is required to calculate the SST anomaly and to determine the occurrence of marine heat waves. It consists of a NetCDF file providing, for each calendar day, the expected SST distribution (i.e., the climatological values), and the 90th percentile values for temperature across the area of interest. This agrees with the methodology described in Hobday *et al.* (2016), which has been followed here, where a marine heat wave is defined as any event characterised by a seawater temperature anomaly exceeding the 90th percentile threshold for at least 5 consecutive days. A suitable SST product needs to be selected. Here, the global Multiscale Ultra-High Resolution (MUR) SST product (Chin *et al.*, 2017) has been selected due to its high resolution (0.01°) coverage of the world ocean, which makes it suitable for standardisation and applications of these best practices in other parts of the world. However, different SST products may be preferred. In any case, the selected product should be used both for preparing the climatology and for displaying the daily SST on the website application (Figure 8), because then the SST anomaly can be easily calculated by subtracting the SST climatology to the actual SST distribution.

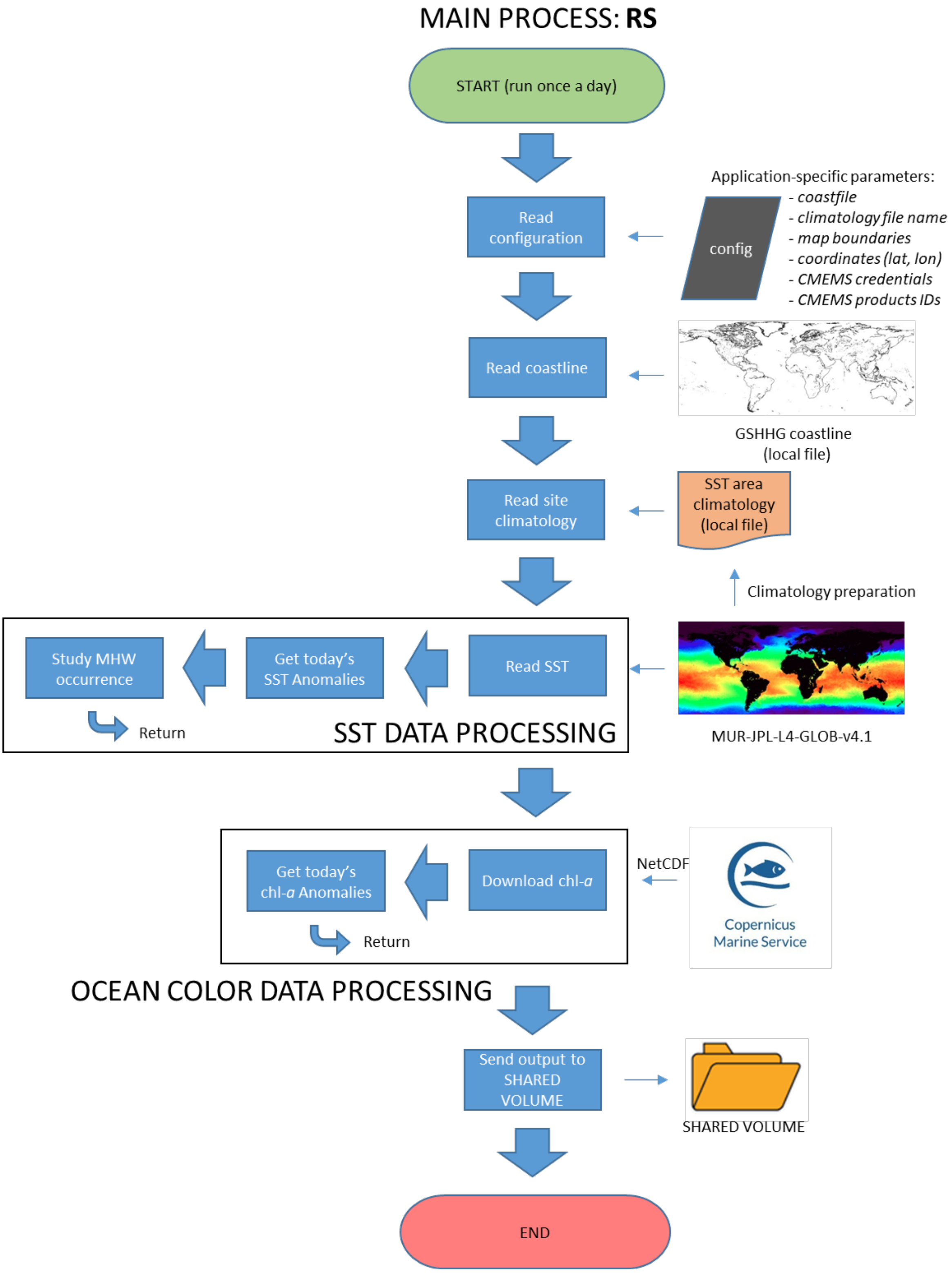


Figure 8. Flowchart describing the remote-sensing data operations.

Chlorophyll-*a* concentration is derived from satellite imagery. The distribution of chlorophyll-*a* concentration is downloaded from ocean colour products available at the Copernicus Marine Service. Then, chlorophyll-*a* anomaly (Figure 9) is determined as the difference between the actual chlorophyll-*a* concentration and a 60-day running median, ending two weeks before the current image (Tomlinson *et al.*, 2004). Tomlinson *et al.* (2004) used a 60-day running mean to calculate chlorophyll-*a* anomalies and investigate the occurrence of *Karenia brevis* HABs in the Gulf of Mexico. The same procedure has been followed here but using a 60-day running median instead, since the median, being less affected by outliers and skewness, is a more robust measure of central tendency and should be preferred when dealing with non-symmetrical distributions.

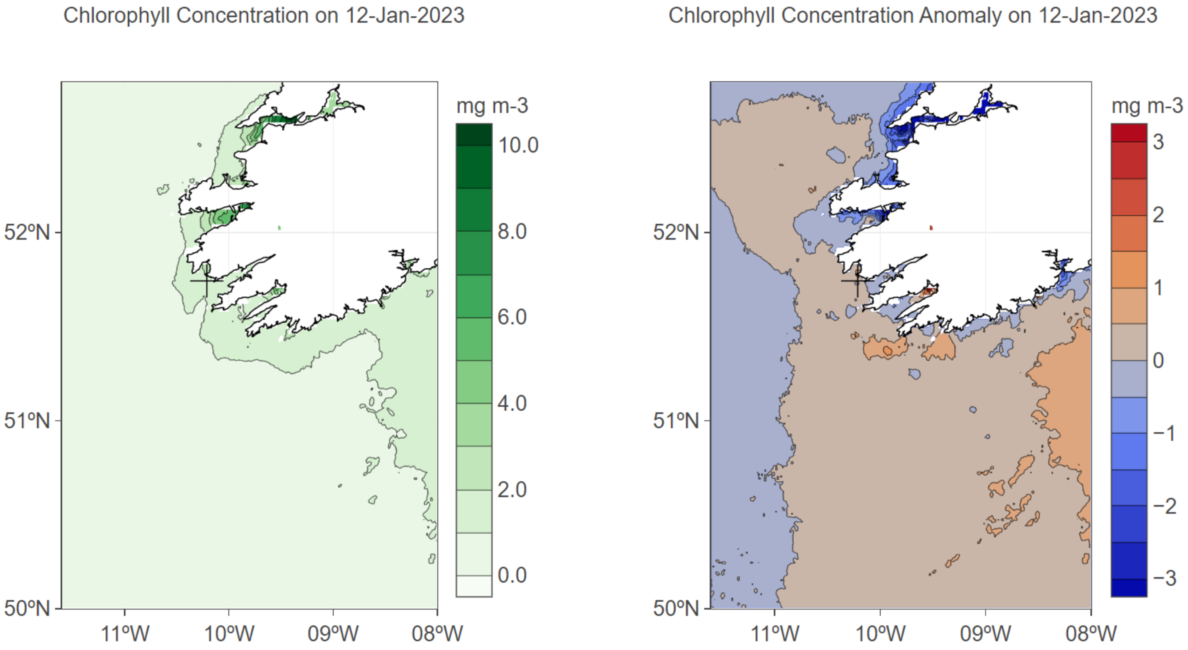


Figure 9. Southwest of Ireland chlorophyll-a (left) and chlorophyll-a anomaly (right) as displayed on the website. The "+" cross shows the location of the Deenish Island farm.

1.3.3.4. Lagrangian Particle-Tracking Model operations: the lptm container

Lagrangian particle-tracking models simulate the advection of water under the influence of oceanic currents. This is useful for a better understanding of the ocean circulation and can be used for tracking of passive tracers in the ocean. More complicated behaviours can be introduced to simulate windage, flotation and degradation, which has applications in the tracking of oil spills, marine litter or floating bodies. Here, particle-tracking modelling is used to track the circulation along the coast to provide insight into the advection of potential Harmful Algal Bloom outbreaks along the southwest coast of Ireland (Figure 10). This part of the application has not yet been implemented for El Campello.

The OpenDrift (Dagestad et al., 2018) particle-tracking model is used. Particles are seeded along four transects on the southwestern coast of Ireland: the *Kenmare* transect, along the mouth of the Kenmare Bay where the farm is located, and three transects perpendicular to the coastline, from west to east: *Dursey*, *Mizen* and *Toe* (Figure 10). A total of 250 particles is released every minute along each transect for 1 day, and each particle is tracked for 3 days. An animation showing the motion of the waters is shown on the data portal.

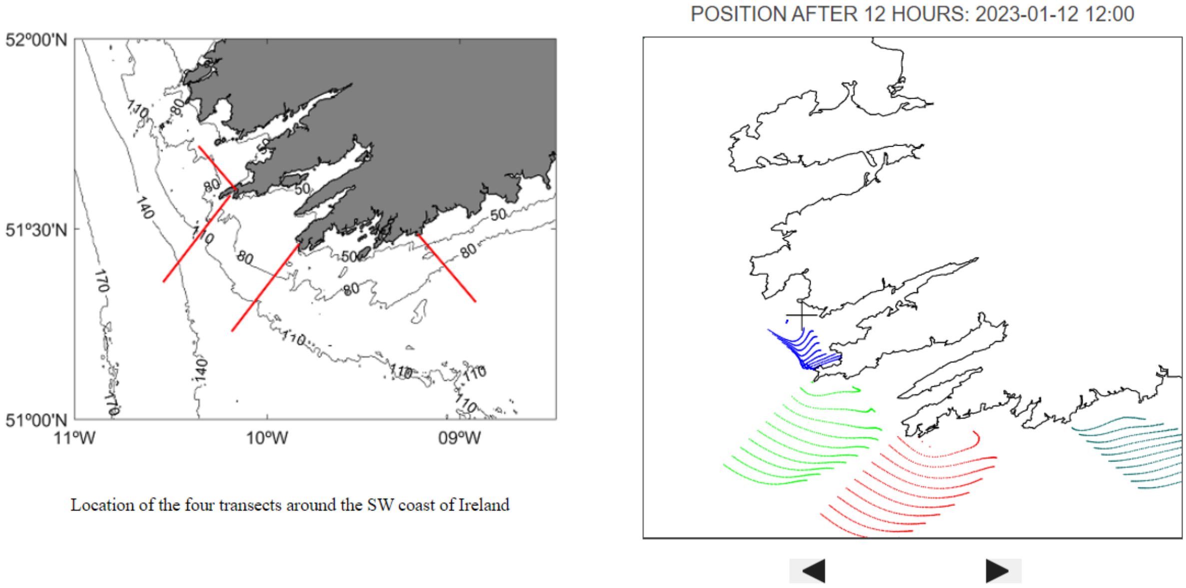


Figure 10. (Left) Transects used as starting sites in the particle-tracking model, from north to south and from west to east: Kenmare, Dursey, Mizen and Toe. (Right) Advection of seawater after 12 hours starting from the transects, as displayed on the website. The "+" cross shows the location of the Deenish Island farm.

In this process (Figure 11), the configuration settings include the specification of the map boundaries (West, East, South, North), the number of particles released per transect and the location of the transects. After reading the configuration settings, the software accesses the 3-day forecasts of oceanic currents delivered by the Marine Institute's Northeast Atlantic model (Dabrowski *et al.*, 2014), a ROMS-based hydrodynamic model covering the waters around Ireland and the Northeast Atlantic with 1.1-2.4 km of horizontal resolution. Hourly instantaneous outputs of this Northeast Atlantic model are freely accessible through a THREDDS server, which makes this product especially suited for this application. Different open-access, highly resolved hydrodynamic models would have to be selected for applications in other regions.

Additional configuration settings are then introduced in the model. Particles are allowed to return to the water even after hitting the coast. Then, particles are released along the transects and the OpenDrift model is run. Finally, the output is sent to the shared volume to be accessed by the application.

1.3.3.5. Deploying the website: the webapp container

The web application provides two distinct functionalities: the Operational (Forecasting & Warnings) System, and the Historical Portal (Figure 12). The former provides the latest observations (*in-situ* + remote-sensing), forecasts and warnings, and feeds on the information provided by the processes described in Sections 2.3.1-2.3.4 above. The latter provides a data selection tool for inspection of older, observed data: the user submits a request consisting of a starting date and an end date, and then the application retrieves the data corresponding to the requested time span. This involves accessing the historical *in-situ* data record prepared by the *site* process (Section 2.3.1.h) or downloading remote-sensing or modelled seawater temperature profile data from other sources, such as the Copernicus Marine Service.

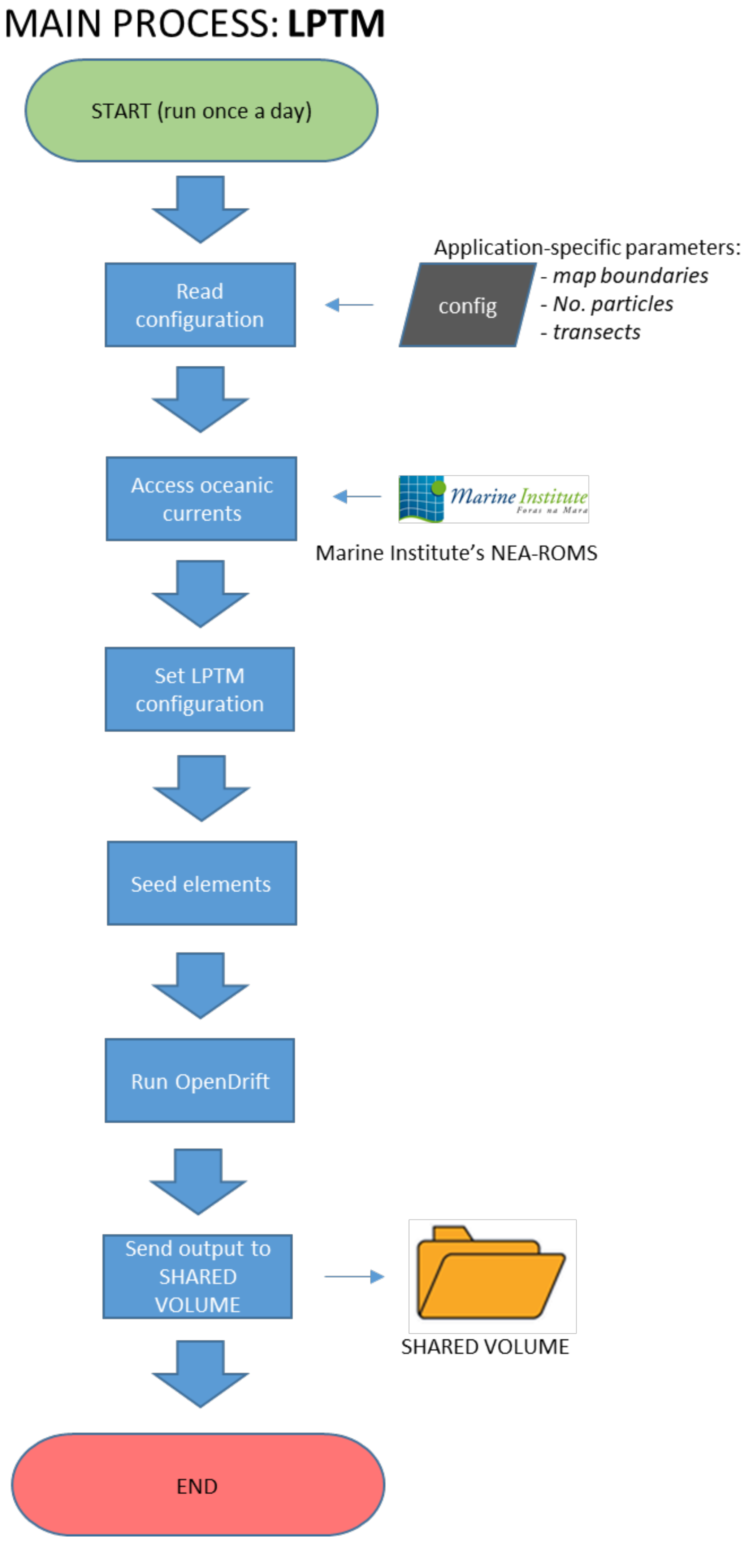
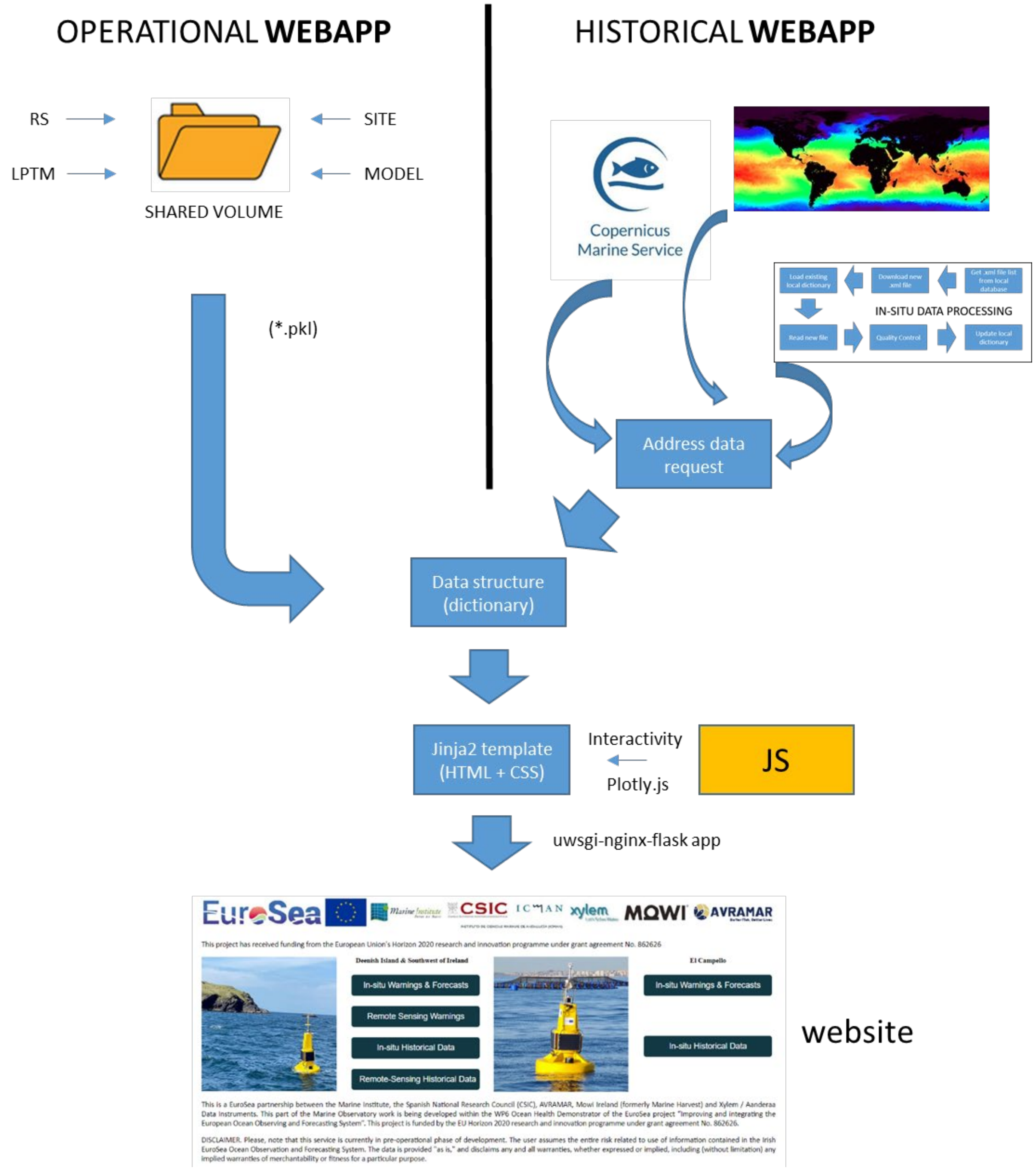


Figure 11. Flowchart describing the Lagrangian Particle-Tracking Model operations.

If the Operational or the Historical functionalities are used, the data that will be displayed on the website are wrapped in a data structure or Python dictionary, that is then sent to a Jinja2 template. Interactive Plotly graphics and other forms of interactivity are achieved using Javascript. Finally, the website is deployed as a uwsgi-nginx-flask application.



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DISCLAIMER. Please, note that this service is currently in pre-operational phase of development. The user assumes the entire risk related to use of information contained in the Irish EuroSea Ocean Observation and Forecasting System. The data is provided "as is," and disclaims any and all warranties, whether expressed or implied, including (without limitation) any implied warranties of merchantability or fitness for a particular purpose.

Figure 12. Flowchart schematizing the web application deployment.

1.3.4. Data Required

The data required to deliver all the outputs available at the website can be listed as follows:

a. The most important dataset is, of course, the ***in-situ* observations** recorded by the monitoring station. For each site, this consists of a set of XML files released every 10 minutes and delivered through an SFTP server hosted by enoc.puertos.es. These XML files contain the readings of each of the sensors in the monitoring station, including the Motus Wave Sensor (significant wave height [m], wave peak direction [Deg.m], wave peak period [s]), the Doppler Current Sensor and Doppler Current Profiler Sensor (horizontal speed [cm/s] and direction [Deg.m]), the Gill Maximet (wind speed [m/s] and direction [Deg.m]), and the YSI EXO2 (Deenish) & YSI EXO3 (El Campello) sensors (temperature [degC], salinity [ppt], dissolved oxygen saturation [%], turbidity [FNU], chlorophyll [RFU] and pH).

b. **Models** providing forecasts and a temperature profile. There are two types of forecasting models that are considered here: **(a) Numerical models**. Hydrodynamic models approximate the mass, heat and momentum conservation equations of the ocean using finite difference methods and, by providing appropriate forcings (i.e., atmospheric and freshwater discharge) and adequate boundary conditions, can predict the evolution of the ocean starting from given initial conditions. Currently, hydrodynamic models provided by the Copernicus Marine Service are being used to provide forecasts and temperature profiles at the aquaculture sites: Met Office's Atlantic – European Northwest Shelf – Ocean Physics Analysis and Forecast in Deenish Island; and the Euro-Mediterranean Center on Climate Change's Mediterranean Sea Physics Analysis and Forecast in El Campello. **(b) Machine Learning models**. In recent years, machine learning techniques, and more specifically neural networks have shown significant results for time series forecasting, given their non-parametric nature, highlighting their ability to approximate continuous and nonlinear functions. Traditionally, models like ARIMA (Ho and Xie, 1998), moving average or exponential smoothing were used to predict future values based on historical data. However, recurrent neural networks like Long Short-Term Memory, LSTM (Yu *et al.*, 2019) or other newer models like Transformers (Wolf *et al.*, 2020) are currently being implemented given their improvements in forecasting efficiency. For example, LSTM models are able to contextualise when working through input and output time series, i.e., understanding how past events condition the upcoming values. In this sense, multivariate time series results are especially interesting when predicting co-dependant oceanic variables, allowing neural networks to learn the relationships between them and thus being able to predict how they will covariate in the future.

c. **Remote sensing.** The aquaculture farmers may be concerned not just by local oceanic processes, but also by the wider oceanographic conditions in the area around the farm. An example is the occurrence of algal blooms that can originate in a remote location and then advected by currents towards the farming area. Remote-sensing products are used to complement the local *in-situ* and model datasets, and to extend the capabilities of this service to a broader area, thus providing information on these wider oceanographic phenomena. Sea surface temperature (SST) and chlorophyll concentration products are being offered for areas covering from 50.0 °N, 11.6 °W to 52.8 °N, 8.0 °W for the Southwest of Ireland waters; and from 37.6 °N, 0.9 °W to 41.0 °N, 1.4 °E for the Levante waters. The SST product is the global Multiscale Ultra-High Resolution (MUR) SST product (Chin *et al.*, 2017). Chlorophyll concentration and anomalies for the North Atlantic is derived from ACRI's Atlantic Ocean Colour (Copernicus-GlobColour), Bio-Geo-Chemical, L4 (daily interpolated) from Satellite Observations (Near Real Time) available from Copernicus Marine Service.

d. **Baseline climatology.** A sea surface temperature baseline climatology has been determined from the 2002-2022 data from the global Multiscale Ultra-High Resolution (MUR) SST product (Chin *et al.*, 2017). The baseline climatology has been determined both for the farming sites (local climatology) and the wider remote-sensing areas (2-D climatology). These datasets are stored in static files that are later used for determining the occurrence of marine heat waves following the definition in Hobday *et al.* (2016). The local climatology is a Python pickle file containing the multi-year mean SST and 90th percentile for the farming site for each day of the year, with a time list ranging from 1 to 366. Examples for Deenish Island and El Campello can be found in the GitHub repository of the project at https://github.com/IrishMarineInstitute/EuroSea. The 2-D climatology is a NetCDF file providing the same information over the same time list, but for a range of longitudes and latitudes covering the area of interest.

e. **GSHHG coastline database**, used for drawing the coastline in the remote-sensing and particle-tracking maps. This is a public dataset (Wessel and Smith, 1996) that can be subset for any region of interest. In this application, the coastlines of Southwest of Ireland and Levante have been downloaded and saved as static, Python pickle files that are accessed by the application. Examples of the expected format of these files can be requested to the developers, as they are not available in the GitHub repository.

f. The Marine Institute's **Northeast Atlantic model** (Dabrowski *et al.*, 2014) oceanic currents are used as input for the OpenDrift particle-tracking model in the Southwest of Ireland. Different choices of hydrodynamic models are, of course, possible, depending on the application site, but this needs to be conveniently set in the LPTM container (see Section 1.3.3.4).

1.3.5. Tools, models and software used

The web server run consists of a Flask web application in Python that runs with uWSGI and Nginx in a single Docker container. For the website containerization, the tiangolo/uwsgi-nginx-flask image has been used. Docker version 20.10.18 has been used in an Ubuntu 18.04.6 LTS (Bionic Beaver) machine. Python version 3.8 is used across all sub-containers. Graphics on the website are rendered with the latest version of Plotly.js. The OpenDrift model v.1.10.4 (Dagestad *et al.* 2018) is used for particle-tracking modelling. The Copernicus Marine User Support Team's motuclient v.1.8.4 is used to download model and remote-sensing data from the Copernicus Marine Service. Additional required Python packages are: netCDF4 v.1.5.7, numpy, pandas, paramiko, pysftp, python-dateutil, pytz, WebOb.

1.3.6. International Standards used

Data Management follows IODE Data Management Quality Framework practices.

1.3.7. Quality Control

Quality Control operates on the *in-situ* observations and consists of detecting abnormal values, outside of naturally occurring intervals, that clearly correspond with missing records, and replacing those values with NaN (Not a Number), so that they are filtered out and not displayed on the website.

1.3.8. Implementation challenges or issues

Possible challenges or issues that may arise during the implementation of these best practice guidelines are:

a. **Data transmission from the monitoring station is stopped.** Oceanographic buoys are exposed to a wide range of weather conditions that may result in severe damage of the electronics and sensors. This will result in a data gap that the web application will have to handle until the instruments are repaired and deployed back into the water. Replacing missing records with a "NaN" value and displaying N/D on the web portal indicate the lack of measurements. Adding a warning message on the home page is advisable to keep users informed.

b. **Unavailability of forecasting data for a particular site.** Forecasts are derived from either hydrodynamic and biogeochemical models, or using a Machine Learning approach (see Section 1.3.4). When none of these approaches are available, forecasting is not possible and the portal only provides access to historical and current conditions.

c. **Establishing a baseline climatology for sea surface temperature** can be difficult due to either (1) lack of a long-term record of sea surface temperature at the site, or (2) lack of confidence on available sea surface temperature records. In the absence of long-term in-situ records, a common approach is to use remote-sensing SST products. However, the existence of biases between the SST record and the actual seawater temperature at the site needs to be taken into consideration. Another subject that has been under debate in EuroSea (Annual Meeting 2022, Cádiz, Spain – Workshop 4A Marine heat waves – a cross-cutting indicator in EuroSea) is the record length used for the computation of the baseline climatology. Hobday et al. (2016) recommends at least a 30-year SST record. However, it has been argued that, since climate change is increasing seawater temperature worldwide, a long SST record could result in an "outdated" baseline climatology, not representative of the current climate. Changes in the choice of baseline climatology can have a large impact on the number, duration and intensity of the marine heat wave warnings provided in this service.

d. Similar to the above, **lack of confidence in the forecasting products**. Whether numerical or statistical approaches are used for forecasting, thorough validation against actual observations is a must to ensure that good-quality forecasts and warnings are being provided.

1.3.9. Visualisation Tools

The information is accessible to the user through an open-access portal at https://eurosea.marine.ie. From the home page, the user can access the different products available for both sites: Deenish Island and El Campello. Available products are either *in-situ* or remote-sensing, and either operational (latest + forecast) or historical. The home page also provides access to the feedback reporting tool, which is described in detail in Section 1.3.9. below. Dedicated portals exist for each site at https://eurosea.marine.ie/Deenish and https://eurosea.marine.ie/Campello.

In the *in-situ* operational portals, latest recorded data and marine warnings are presented at the top of the page for a quicker and more convenient access. Point data are displayed as time series, whereas 2-D data are displayed with colour contour plots. Care was taken to choose a colour blind-friendly palette.

Graphics are rendered using Plotly.js because it provides useful interactive tools, such as the individual data display when hovering the mouse pointer over the time series and 2-D contour plots. For a more detailed examination of the data, downloading options are available to the user. When a download request is submitted, a CSV (Comma-Separated Values) file with the data being displayed is automatically downloaded to the user's PC. Currently, this downloading functionality is only available for time series, but not for 2-D maps.

Further interactivity on the website is achieved with Javascript for (a) selecting the temperature profile layers that the user wishes to visualise, and (b) forward and backward moving along a Lagrangian particle-tracking simulation.

1.3.10. User Feedback Mechanisms

User feedback is of paramount importance throughout the whole process to ensure that the service addresses the stakeholders' needs and concerns in relation to the aquaculture activities. User feedback is gathered through three different mechanisms:

a. **Direct, periodic, face-to-face interaction.** This is achieved through periodic meetings (either in person or online) arranged periodically at times that are convenient for both stakeholders and developers. The meetings should focus on the interests and needs of the farm, and how this has been addressed by the portal. Discussions may relate to different aspects of the service, such as:

- What type of information is being displayed? What ocean parameters are of greater concern for the stakeholders? (e.g., seawater temperature, dissolved oxygen saturation, wave height, etc.) What type of products need to be considered? (*in-situ* data, remote-sensing, model forecasts, etc.). *Example: Mowi, growing salmon in Deenish Island, is mostly concerned about the occurrence of high seawater temperature events at the farm. Therefore, current and forecasted temperature should be displayed at the top of the website. Not just the in-situ temperature measured by the buoy, but also the temperature profile across the water column is relevant in this application, since the salmon cages spread several metres deep. A model is used to provide an estimation of the water temperature profile. Furthermore, remote-sensing SST is provided to inform about the seawater temperature distribution on a wider area covering the Southwest of Ireland. On the other hand, AVRAMAR, growing gilt-head bream among other species in El Campello, is not concerned about seawater temperature since this species is tolerant to the warm Mediterranean waters. Rather, their main concern is severe storms making it difficult to work at the sea, and thus the current and forecasted wave height has to be displayed at the top of the website.*
- What is the most appropriate appearance of the graphics for a clear and understandable visualisation? Aspects like font size, colour blind friendly palettes or adequate number of contours in 2-D colour maps need to be considered so that the information is clear to everybody.
- What type of warnings are relevant to the farming activity? This largely depends on the stakeholder needs and the physiological requirements of the species grown in the farm. Are environmental conditions affecting fish health of greater concern? Is the species sensitive to rapidly changing environmental conditions or extreme marine events, or is it tolerant to a wide range of oceanic conditions? Are weather conditions affecting work and safety at sea the greatest concern? This is similar to what has been discussed above.
- What is the frequency at which the information should be updated on the website? Hourly? Daily?

User feedback collected during these meetings is then used to improve the service towards a new version that is closer to the stakeholders' expectations, and before a new meeting takes place. This process is repeated in an iterative manner until the final product is achieved.

b. **Questionnaires.** Over the course of several months after the deployment of the service, end users are requested to complete questionnaires reflecting their experience interacting with the website, consulting their opinion on different aspects related to the usefulness, friendliness and ease of use of the portal. These questionnaires are useful to determine the degree of satisfaction of the stakeholders and the feedback gathered is used to improve the service.

c. **Feedback reports.** The website includes a free-text input field at https://eurosea.marine.ie/reporting-feedback to provide any feedback at any time on aspects related to the user experience. When the users click the "Submit" button, a plain text file is sent to the developers, and this file is treated as a feedback report that is then considered for future improvements of the portal. This provides an easy and alternative mechanism of providing feedback on the service besides the meetings and questionnaires.

2. Conclusions

This work presents initial best practices guidelines to follow when deploying an online, open-access marine observatory serving the needs of the aquaculture sector. *In-situ* observations, remote-sensing data and model forecasts and warnings are rapidly consulted through the application described here. This Version 0.1 BP will hopefully serve as a good demonstrator that is useful for others looking to develop similar applications for aquaculture in other parts of the world.

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