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A Web-Based Observatory for Biogeochemical Assessment in Coastal Regions

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ABSTRACT. The concept of water observatories is extended to create a highly versatile tool for both the daily and the long-term management of estuarine ecosystems. Coastal observatories are evolving from simple data repositories to include forecasts, scenarios' analyses and indicators, integrated in web platforms that provide multiple products and services. In a context of climate change (CC) and growing anthropogenic pressures, the assessment of the ecological health implies that the biogeochemical status is adequately quantified and incorporated in the coastal management decision-making procedure. This quantification requires accurate models for hydrodynamics and ecology that account for all relevant processes at the right scales. These models must be applied in forecast mode for emergency purposes and in hindcast mode to explore multiple scenarios as part of the CC adaptation strategy, creating a complex, vast amount of information to be shared with the coastal managers. A web-based portal supported by a comprehensive modeling and forecasting framework and materialized along the main water quality/biogeochemistry themes, from data to indicators, is developed and demonstrated in two distinct yet complex coastal systems: the Tagus estuary and the Ria Formosa lagoon. The paper starts with the requirements analysis from both ecological and computer science perspectives and then presents the overall multi-layered architecture of the framework and its key software components. The observatory portal implementation and demonstration explore its usefulness for coastal management.

Keywords: biogeochemistry, numerical modeling, real-time data, forecast framework, web portal, information repository, estuaries and coasts, Tagus estuary, Ria Formosa

1. Introduction

Estuaries and coastal lagoons are among the most productive ecosystems on Earth and provide multiple ecosystem services (e.g., Barbier et al., 2011; de Groot et al., 2012). They harbour ecologically important habitats for fish, shellfish and birds, and, due to their buffering capacity, protect the coastal ocean from increased nutrient loads and other terrestrial contaminants (Cloern, 2001; Paerl, 2006). These coastal systems also support diverse human activities (e.g., marine transportation, fishing, tourism, and are repository waters for domestic wastewater), providing economic resilience to coastal communities and protecting them from natural and anthropological hazards. However, over 400 coastal systems worldwide have been identified as eutrophic or hypoxic areas due to a significant growth of nutrient loadings from terrestrial anthropogenic activities (Selman et al., 2008). The growing human activities in coastal areas (Rabalais et al., 2009) and climate change (CC) may increase the hazards in these systems (Statham, 2012), and alter the ecosystems dynamics. CC effects, such as sea level rise, represent a major threat to the world's estuaries, via potential changes in the hydrologic regimes, increases in salinity, acceleration in the nutrient cycling and disruption of aquatic ecosystems (Pethick, 2001; Statham, 2012). Also, recent and predicted increases of nutrient loads to coastal systems (Rabalais et al., 2009) may exacerbate the impacts of CC. These impacts may reduce the regulating services provided by the coastal systems, which value was estimated at about 25,000 International$/ha/year (2007 price levels; de Groot et al., 2012). Thus, assessing how human-induced or climate drivers threaten the estuaries and coastal lagoons is fundamental for the daily and the long-term management of these water bodies (Paerl, 2006), as it can support the establishment of protection measures and foster better-informed decision-making.

Several data-based or model-based studies aimed to evaluate the physical and biogeochemical dynamics in coastal systems (e.g., Cravo et al., 2014; Romero et al., 2019; Dan et al., 2019; Rodrigues et al., 2019; Suari et al., 2019; Aveytua-Alcazar et al., 2020). However, integrated studies that assess both climate-driven and anthropogenic-driven scenarios and management approaches combining the potentialities of numerical modelling and data analyses remain scarce (e.g., Rodrigues et al., 2015b), mainly due to the challenge of integrating different sources of information that cover the relevant temporal and spatial scales. In this context, coastal observatories can be effective tools to overcome some of these challenges.

Coastal margin observatories are fundamental components of management in coastal regions (e.g., Baptista, 2006;

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Baptista et al., 2015; Fortunato et al., 2017a; Fennel et al., 2019), as they offer the flexibility to handle both early-warning and long-term planning and to easily access large amounts of disparate data. These systems can comprise several layers of information, including the provision of historical and real-time monitoring data, hindcasts, short-term forecasts and scenarios. Crossing different temporal scales, coastal observatories enable: i) the identification and understanding of shifts in the systems by providing long time-series of environmental data, ii) the anticipation of hazardous events by providing forecasts of water conditions (e.g., water levels, temperature), and iii) the assessment of future trends (e.g., in response to CC) through the analysis of available simulations of scenarios.

Although there are worldwide many detailed and broad-scope monitoring systems of the ecological status of coastal systems (e.g., the LTER network, https://lternet.edu/), linking data with physical-biogeochemical models is necessary to achieve a thorough understanding of the coastal dynamics in a context of CC and growing anthropogenic pressures. Coastal observatories, combining numerical models for physical processes (e.g., water levels, waves) and monitoring data, are relatively well-established tools (e.g., Fortunato et al., 2017a), but operational systems for assessing the biogeochemical status of coastal waters are still in their infancy (e.g., Fennel et al., 2019). On the one hand, numerical models, which simulate the physical and biogeochemical processes at the relevant spatial and temporal scales, are useful tools to complement the data and to exploit the ecosystem's response to different scenarios (e.g., Megrey et al., 2007; Charria et al., 2016; Rodrigues et al., 2019). On the other hand, consistent data facilitate model validation and provide complementary means to investigate ecosystem evolution. Implemented in operational frameworks, integrated data-model approaches offer a continuous surveillance of the systems, allow the adjustment of existing monitoring strategies and provide a valuable repository of data and model predictions to support coastal management and science.

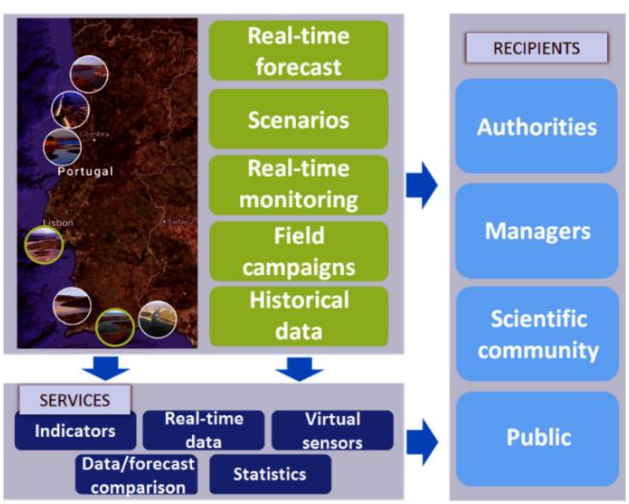

Figure 1. Overall concept of the UBEST observatory and location of the application sites (Tagus Estuary and Ria Formosa).

Thus, this study aims to develop and demonstrate a new coastal observatory, the UBEST (Understanding the biogeochemical Buffering capacity of ESTuaries) observatory, to assess the biogeochemical status of coastal systems. This observatory integrates several layers of information, from real-time data and forecasts to indicators, in a user-friendly web portal. It is demonstrated in two Portuguese coastal systems, the Tagus estuary and the Ria Formosa (Figure 1).

The paper is organized as follows. Section 2 provides a general description of the concept and requirements of the UBEST observatory. Section 3 describes its architecture and building blocks. Section 4 illustrates its applicability at the coastal sites to: i) support the long-term management in the Tagus estuary and, in particular, assess the nutrient status in this estuary and the estuary response to CC, and ii) support the daily management in the Ria Formosa and, in particular, perform real-time monitoring and provide forecasts of the water quality in the lagoon. The main conclusions are presented in Section 5.

2. The UBEST Observatory

2.1. Concept

The UBEST observatory aims at empowering the users to answer their own questions on a particular coastal system. These questions can have a broad scope. The user may ask questions related to the long-term behavior of the system. What is the physical or ecological status of the system? How has this status evolved over the past decades? Did it respond to a particular change in inputs? Does it exhibit seasonal patterns? How will it evolve in different scenarios? Or the user may have a narrower focus and ask questions on shorter time or spatial scales. Will the water quality change tomorrow due to an expected weather change? Are there spots in the estuary where water quality problems are more acute?

Users may have different levels of understanding of the processes. Hence, the observatory should provide information at different levels of aggregation. For instance, some users may want to look at time series of the basic variables, others may only want to examine their statistics, while others still may want to examine a higher level of aggregation through indicators based on several variables. Also, users may want to explore the answers with different datasets. Therefore, the observatory should provide information of different sources, namely both field data and model results.

The type of questions illustrated above are often addressed by contractors, and provided to the water authorities in the form of technical reports. However, advancing from the question to the answer requires finding funding, preparing formal tending procedures and performing the studies. Hence, the time lag between the question formulation and the report delivery can vary from months to years. Observatories can drastically reduce this time lag. This reduction should foster more questions, facilitate the involvement of more stakeholders, and ultimately lead to better and more timely decisions.

The approach used to build the UBEST observatory relies on the concept of a user-friendly web portal that provides several layers of information, with different levels of aggregation

(Figure 1) including: i) historical data, ii) real-time data from monitoring networks, iii) daily forecasts of physical and biogeochemical variables simulated with operational models, iv) simulations of scenarios of climate change and anthropogenic pressures, and v) indicators that summarize both the physical behavior and the water quality status of the systems. Moreover, this observatory is easily customizable, so other coastal systems can be easily added to the observatory portal. The main requirements to build the UBEST observatory and its main properties are described below.

2.2. Requirements and Main Properties

Existing coastal observatories are typically field data repositories of distinct data sources where data can be combined to produce new information and address specific concerns of the system of interest (for example the observatories provided in the research infrastructure Jerico Next, presented in Puillat et al., 2016; or LTER observatories, as described in Suari et al., 2019). Model hindcast and forecast products are not frequently integrated with these data hubs. Even within the modeling community, a separation is made between short and long-term products. Forecasts are typically made available through interfaces dedicated to operational, short-term management (Fortunato et al., 2017a), while model hindcasts are shown in portals for long-term concerns, such as CC impacts (e.g., Durrant et al., 2013) or anthropogenic action effects (e.g., building of a new infrastructure in the coastal zone). Hindcasts are also used to support data-driven analysis, for instance to extract information for tailored scientific questions such as in the work of Charria et al. (2016). Some exceptions combine forecast and hindcast products, for instance in a risk management context (Gomes et al., 2015), but data are only included for model validation.

In UBEST, a new concept of observatory was required, seamlessly integrating field data, scenarios and forecast products to provide the best information calculated with field data and model results. The UBEST observatory should be an observatory-building service that accounts for the several requirements and characteristics of any type of coastal system, and targets the specific portal products to the site characteristics. Based on the experience from previous projects (Gomes et al., 2015, Oliveira et al., 2020) and from other works based on hindcast model platforms (Oke et al., 2015), it should be therefore supported by a site-independent numerical model and a flexible computational infrastructure that can be used to generate observatories for new sites in a simple manner.

This new concept of observatory poses several challenges and demands several properties from an information technology (IT) perspective for both users and administrators. These properties of service are listed below along with a short explanation on the implementation choices:

1. Global accessibility: the observatory portal should be easy to access on every device. Choice was made to use a web portal, which does not require additional configuration or software installation.
2. Comprehensiveness: the observatory portal should be able to tackle all relevant problems and provide a one-stop-shop for all relevant products adapted to each system characteristics. It should also provide the ability to handle data integration, processing and visualization.
3. Independence: the portal should be self-contained in terms of installation, minimizing dependencies on external software that can reduce its robustness and limit its use. The portal should also be based on open-source software, to reduce dependencies on software licenses and associated costs which may also limit its broad application.
4. Flexibility and ease of maintenance: from an administration perspective, integrating the Django web framework (Django, 2020) within the portal allows taking advantage of its automatic administration interface that provides simple and straightforward management of users and site observatories and all their properties, as well as accounting and quality control tasks.
5. Accuracy: the quality of model results depends directly on the accuracy and robustness of the model being used for the simulations. Herein we use SCHISM (Zhang et al., 2016), an open-source, unstructured-grid, high performance modeling suite, supported by a strong international community and with widespread use for both hindcast and forecast purposes.
6. Modularity and ease of extension: ecosystem modeling and data processing, in particular in the scope of artificial intelligence, can still be improved from current knowledge. Therefore, the capacity to grow and adapt to new algorithms and indicators is an important feature in an observatory platform. Therefore, UBEST was built applying a modular strategy. This strategy constitutes a core property to support the growth of the observatory and the adaptation to the best available knowledge.
7. Simplicity and usability: the portal should provide a straightforward experience to users, regardless of their experience with computational tools. UBEST allows both inexperienced and experienced users to analyze data and model products and to assess compliance to directives through its indicators. Transparent integration to the Portuguese National Infrastructure for Distributed Computing for both everyday forecasting and on-the-fly calculations at the web portal is a particular asset of UBEST that contributes to an adequate interface performance.

2.3. Overall Architecture

The UBEST observatory portal (http://portal-ubest.lnecpt/) has a web portal, which provides detailed information to the user about the water conditions in a given coastal system, and the associated services, which provide that information, namely the data repository and the WFS/WMS map server (Figure 2).

The web portal is developed in Django, a Python web framework aimed for full-stack web development. Thus this web portal has a Frontend, where the web framework provides the HTML pages for the user interactions, and a Backend (with PostgreSQL Database), where the web framework processes the user requests (Figure 2), such as page loading or data fetch, and the web portal data are stored on the database. Other technologies are applied on the Frontend pages, such as Openlayers (map viewer) and Javascript (web scripting language). The following dashboards compose the UBEST web portal:

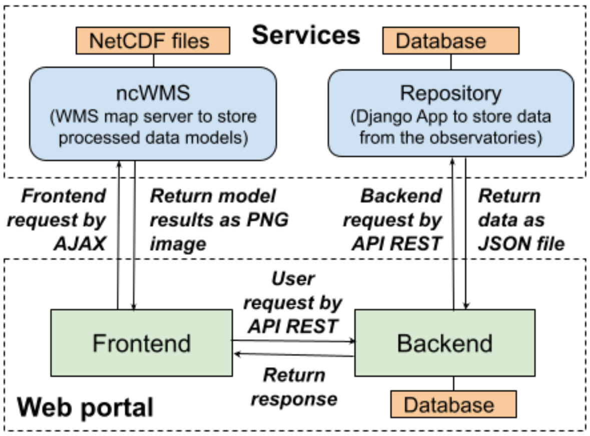

Figure 2. Architecture of the UBEST observatory portal.

- 'Today' (Figure S1) is an operational dashboard that presents a snapshot of the current state of the coastal system, which embeds all the available data and forecasts for the current day; this dashboard is easily configurable by the users for their particular interests, providing mechanisms to show or hide the features that they wish to see;
- 'Data' (section 2.4.1) gives the user the ability to access, view and download field data at all available stations;
- 'Forecasts' (section 2.4.2) displays a 48-hour forecast of physical and biogeochemical variables from operational models;
- 'Scenarios' (section 2.4.3) presents the system's susceptibility to CC or anthropogenic pressures scenarios through hindcast model simulations results;
- 'Indicators' (section 2.4.4) provides synthesized information using indicators for the circulation and water quality status that allows the user to assess possible changes in the coastal system dynamics and biogeochemistry.

The UBEST observatory portal relies on information available from the data repository and the WFS/WMS map server. The data repository (section 2.4.1) provides data from several stations, obtained by in-situ sensors that measure different variables and automatically upload them in real-time by internet to the repository. The repository is also used to store and provide historical field data from in-situ observations and some data derived from both observations and model results (e.g., indicators). The WFS/WMS map server is automatically fed by daily operational simulations (section 2.4.2) and provides information for the Forecasts, Scenarios and Indicators pages.

Regarding the dependent services (Figure 2), requests to fetch data directly from the WFS/WMS map server (model results) are made on the Frontend, while requests to fetch data directly from the repository (monitoring data and indicators) are made on both the Frontend and the Backend. To fetch the models' results from the WFS/WMS map server, the page (Frontend) sends a Javascript AJAX request to the ncWMS (Blower et al., 2013) service to obtain an image of the model results that can be loaded to the page as a layer on the map viewer. To fetch data from the repository, the page (Frontend) sends a Javascript AJAX request to the Backend, which sends another request to the repository to return the JSON data back to the Frontend.

2.4. Building Blocks

2.4.1. Data Model and Data Infrastructure

The UBEST coastal observatory keeps its data in the repository, a web-based application supported by a relational database. The application is built on the Django web framework, modeling a simplified version of the Observation Data Model 1.1 design specification (Tarboton et al., 2008), and backed by a PostgreSQL (PostgreSQL, 2020) relational database management system.

The Data Model (DM) allows a detailed characterization of the data, as most models (data entities) describe meta-information related to actual measurements or results. Such models contain curated information about important aspects, like location (Site), collection (Dataset), among others (see Figure S2 of Supplementary Material). ScalarValue and the optional ScalarValueTideDetails models hold all the actual measurements or results.

The repository application contains only the essential components (apps in Django world) to fulfill its purpose, namely datamodel, gateway and importer. The datamodel implements the DM, which stores all the data and facilitates basic management through the Django's built-in administration portal. The gateway provides the means to fetch most data conveniently via a REST API. Finally, the importer offers several ways to load data into the repository, from local CSV files to specific probes, including a mini framework to simplify the addition of new methods.

The user can access the repository field data through the 'Data' dashboard. Data available are organized in several physical (e.g., water levels, salinity), chemical (e.g., dissolved oxygen, ammonium, phosphate, pH) and biological (e.g., chlorophyll a) variables. The 'Data' dashboard allows the user to search and filter stations with available data by variable, value condition, date and/or water body. After selecting at least one station on the map, a pop-up is shown that provides several functionalities, including charts of the selected variables (that can be exported as image files) and a 'View/Export Data' menu that lists the data and allows the user to export it as a csv file. The 'Data' dashboard also provides statistics of the data available at each station.

2.4.2. Forecast Engine

The UBEST forecasts are performed daily, taking advantage of an established model and procedures to reliably and consistently produce the predictions. These procedures are assembled in the forecast engine, a software built on top of the Water Information Forecast Framework (WIFF, Fortunato et al., 2017a; Rogeiro et al., 2018), a Python-based framework, that is also used to enable the on-demand forecast systems in the OPENCoastS service (https://opencoasts.ncg.ingrid.pt, Oliveira et al., 2020). WIFF provides most of the generic aspects required to operate a forecast system, such as coupling different simulation models, retrieving the necessary forcings, running simulations remotely or locally with MPI, chaining periodic simulations to make them a continuous series of events, post-processing the model results and providing notifications to the users and administrators about progress or unexpected behavior. The modularity in this procedure also allows them to be customized and/or extended, by subclassing. Figure 3 depicts the forecasting software stack.

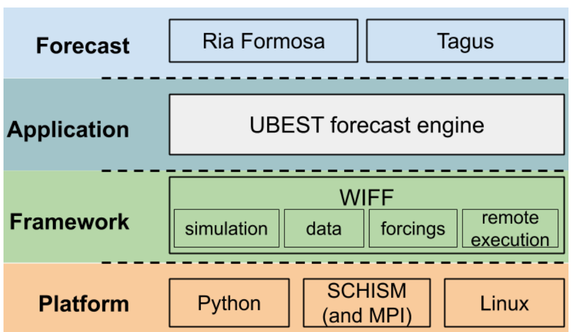

Figure 3. UBEST forecast engine: forecasting software stack.

The UBEST forecast engine's main purpose is to operate the SCHISM model, used to produce daily forecasts for the coastal systems. SCHISM (Semi-implicit Cross-scale Hydroscience Integrated System Model) is a community modeling system based on unstructured grids in the horizontal dimension and hybrid SZ coordinates or LSC2 (Localized Sigma Coordinates with Shaved Cell) in the vertical dimension. This modelling system is fully parallelized and uses semi-implicit finite elements and finite volume methods, combined with Eulerian-Lagrangian methods, to solve the shallow water equations. It includes modules for surface waves (Roland et al., 2012), morphodynamics (Pinto et al., 2012; Guerin et al., 2016) and water quality (Rodrigues et al., 2009, 2011; Azevedo et al., 2014).

The current application of SCHISM in the UBEST observatory comprises the use of the 3D baroclinic hydrodynamic model coupled to the biogeochemical module (Rodrigues et al., 2009, 2012). The hydrostatic version of the model solves the three-dimensional shallow-water equations and the transport equations for salt and heat. SCHISM has a user-defined transport module that allows the simulation of any given tracer through which the biogeochemical module is coupled. The biogeochemical model formulation was extended from EcoSim 2.0 (Bisset et al., 2004) to simulate zooplankton and the oxygen cycle (Rodrigues et al., 2009, 2012). This model includes the carbon, nitrogen, phosphorus, silica, oxygen, and iron cycles and simulates several ecological tracers. Several options are implemented within the model that allows the user to select the relevant variables for a specific application. Further details about SCHISM's physical and numerical formulations can be found in Zhang et al. (2016; core hydrodynamic model) and Rodrigues et al. (2009, 2012; water quality/biogeochemical module).

Forecasts are updated daily based on the information for the forcings at the boundaries. Several forcings are available in the forecast engine to establish the boundary conditions for oceanic, riverine and surface (atmosphere) boundaries. Oceanic boundaries are forced by ocean forecasts, sourced from Copernicus' CMEMS IBI_ANALYSIS_FORECAST_PHYS_005_001 and IBI_ANALYSIS_FORECAST_BIO_005_004 (http://marine.copernicus.eu/), for physical and biogeochemical variables, respectively. Riverine boundaries can be forced by extrapolations of quasi real-time data or climatology. Regarding the surface boundary, atmospheric forecasts sourced from NOAA's GFS 0.25º are used as well (https://www.ncdc.noaa.gov/data-access/model-data/model-datasets/global-forcast-system-gfs). Two-day forecasts are provided for the following variables: water levels, velocity, salinity, temperature, ammonium, nitrate, phosphate, silicate, dissolved oxygen and chlorophyll a.

Forecasts are available through the 'Forecast' dashboard. This dashboard allows the user to: i) view the model forecasts on a map and their evolution by vertical level or by time (48 hours) - 'Access'; ii) view a comparison of today's available field data at the repository with the model forecasts and to view/export these data - 'Model Comparison'; and iii) probe the model results for any selected point in the computational domain and view/export the model forecasts - 'Virtual Sensors'.

2.4.3. Scenarios

The 'Scenarios' dashboard provides information about the coastal system response to scenarios of CC and anthropogenic pressures. The scenarios can address several issues, such as sea level rise, the increase of the air temperature or changes in nutrient concentrations from point sources (e.g., wastewater treatment plants). The scenarios are established for a given coastal system and simulated previously using numerical models. The model results are then made available through the ncWMS services as maps with statistics (means, maxima and minima) of the physical (e.g., salinity, temperature), chemical (e.g., ammonium, dissolved oxygen) and biological (e.g., chlorophyll a) variables. Besides viewing the maps, the user can also see the value of each variable at a selected location.

2.4.4. Indicators

The 'Indicators' page provides synthesized information about the circulation and the water quality conditions in the coastal system. Data are fetched from the repository or the ncWMS services, since the estimations can be evaluated from field data, model forecasts or scenarios, depending on the selected indicator.

To assess the circulation and the mixing conditions the classification proposed by Geyer and MacCready (2014) is used. Geyer and MacCready (2014) developed a classification diagram based on two dimensionless numbers, the mixing number and the freshwater Froude number. Based on the values of those numbers the system can be classified as "Fjord", "Bay", "SIPS - strain induced periodic stratification", "Strongly stratified", "Partly mixed", "Well mixed", "Salt wedge" or "Time-dependent salt wedge". The Geyer and MacCready indicator is automatically computed daily, using a Python script, based on the water levels and velocities forecasts for a given coastal system. Experience indicates that the value of this indicator varies with the choice of the cross-section of the estuary where it is computed. Also, it was derived for estuaries where the flow can be represented by its lateral mean, which may be invalid when the geometry is complex (e.g., due to the presence of lateral bays, various channels or rapid variations in width), as is the case in the two examples used in this study. Hence, the choice of the cross-section should be preceded by a sensitivity analysis, and the selected cross-section should be representative of the main channel, in an area with a slow variation of the cross-section.

Regarding the water quality/biogeochemistry two indicators are available: the chemical status of nutrients based on Caetano et al. (2016) and the Trophic index (TRIX, Vollenweider et al., 1998). Both indicators are computed from historical field data and the TRIX is also computed from the scenario results. The nutrient status indicator was developed for the Portuguese transitional waters and classifies the chemical status of nutrients (ammonium, nitrate + nitrite and phosphate) based on a ratio between nutrient and benchmark concentrations (i.e., [nutrient]:[benchmark]). The 90th percentile of all ratios for a given nutrient is calculated and the final classification is given by the worst score. The quality is classified as "High", "Medium" or "Low" for ratios smaller than 1, between 1 and 2, and larger than 2, respectively. TRIX aggregates the information of four key water quality variables, chlorophyll a, oxygen saturation, dissolved inorganic nitrogen (sum of ammonium, nitrate and nitrite) and soluble reactive phosphorus. The classification is set as: "High" – $0 \leq$ TRIX < 4; "Good" – $4 \leq$ TRIX < 5; "Moderate" – $5 \leq$ TRIX < 6; "Poor" – $6 \leq$ TRIX < 10.

3. Demonstration at Two Coastal Sites

3.1. Long-Term Management of the Nutrient Status in the Tagus Estuary

3.1.1. Study Area

The Tagus estuary, located on the Portuguese west coast, is one of the largest estuaries in Europe with an area of about 320 km^2 (APA, 2016). The estuarine margins are intensively occupied, with a population of about one million inhabitants, and support diverse uses and activities (urban, industrial/harbors, agriculture, shellfish harvesting) and a major natural reserve, which is one of the most important sanctuaries for wintering or staging birds in Europe. There are sharp contrasts in the utilization of the margins: urban and industrial facilities dominate in the right margin, while agriculture dominates in eastern and southern marginal areas (Tavares et al., 2015). The Tagus estuary has a complex morphology, with a deep and narrow inlet channel and a broad and shallow inner basin and an intertidal area of about 40% of the total estuarine surface (Castanheiro, 1986).

The circulation in the Tagus estuary is primarily driven by tides and, to a small extent, by river flow, wind, atmospheric pressure and surface waves (Fortunato et al., 2017b). Tides are semi-diurnal, ranging from 0.55 to 3.86 m at the coast (Guerreiro et al., 2015), and the tidal propagation within the estuary is complex (Fortunato et al., 1997, 1999). The main source of freshwater discharging into the estuary is the Tagus River, with an average flow of 370 m^3/s (APA, 2012). The Sorraia and the Trancão rivers also contribute to the freshwater inflow into the estuary. The estuary is often considered well-mixed, but stratification has been observed at high flow rates and low tidal ranges (Neves, 2010; Rodrigues and Fortunato, 2017).

The heavy industry, the large population and the agricultural exploitation in the margins of the estuary have contributed to several water quality problems in this estuary: contamination by heavy metals (Caçador et al., 1996, França et al., 2005), fecal bacteria (Rodrigues et al., 2015a) and nutrients (Caetano et al., 2016). Here, we focus on the excess in nutrients, since this is a matter of concern for the water authorities when assessing the water bodies status in the context of the European Water Framework Directive.

The spatial and time variability of the Tagus estuary requires information at different scales to provide an accurate view of the ecological status of this waterbody. In addition, because this status depends on several variables, it is easier to provide users with indicators that are able to aggregate information. Finally, models can have significant errors, and field data are normally scarce. Hence, using both sources of information can provide a more complete picture of the status of the estuary.

3.1.2. Model and Scenarios Description

The numerical model of the Tagus estuary extends from the ocean, 27 km away from the estuary mouth, to the river. The horizontal grid has about 83,000 nodes and a typical resolution of 15 ~ 25 m, which is lower in the channels to allow the proper propagation of the tide (Figure S3 in the supplementary materials). The vertical domain is discretized with a hybrid grid with 39 SZ levels (30 S levels in the upper 100 m, and 9 Z levels between 100 m and the maximum depth). The numerical model is forced by: i) tides, salinity, water temperature and water quality tracers' concentrations at the oceanic boundary; ii) river flows, salinity, water temperature and water quality tracers' concentrations at the riverine boundaries (Tagus and Sorraia rivers); and iii) atmospheric data at the surface. The model runs at about 1:4 of real time using 18 cores. Further details about the hydrodynamic model implementation can be found in Rodrigues and Fortunato (2017).

Prior to the implementation of the model in forecast mode, it was calibrated and extensively validated. This validation was performed by comparison of the model results with the several datasets. The datasets included water levels data (Fortunato et al., 1999), salinity and water temperature data (Silva et al., 1986; Neves, 2010), and physical, chemical and biological data from synoptic field campaigns performed specifically for the UBEST observatory (Rodrigues et al., 2020). Some examples of the model results and error measures are presented in the supplementary materials. Overall, the results showed the model's ability to represent the circulation and water quality main spatial and temporal patterns of salinity, temperature, nutrients, chlorophyll a and dissolved oxygen observed in the Tagus estuary (Figures S4 and S5, and Table S1 of Supplementary Material). The main differences between the observations and the model results arise from uncertainties in the boundary conditions and the existence of other point sources that were not considered in the model, namely relative to the input of nutrients (e.g., wastewater treatment plants). Further details about the Tagus estuary hydrodynamic model validation can be found in Rodrigues and Fortunato (2017) and Rodrigues et al. (2019).

The validated hydrodynamics and biogeochemical model was used to simulate several scenarios of climate change and anthropogenic pressures in the Tagus estuary. To establish these scenarios a methodological approach similar to Rodrigues et al. (2015b) was followed. A set of scenarios for conditions anticipated for the end of the 21st century was defined and a reference scenario was established from climatology for comparison purposes. In each scenario only one variable is changed relative to the reference scenario. The following scenarios were simulated for the Tagus estuary:

- Sea level rise (SLR) – this scenario considers a mean sea level rise of 0.5 m. This value was defined taking into account that the median values of SLR between 1986 ~ 2005 and 2081 ~ 2100 depend on the Representative Concentration Pathway (RCP) and that typical values estimated for the end of the 21st vary between about 0.4 m for RCP2.6 and 0.7 m for RCP8.5 (Nauels et al., 2017);

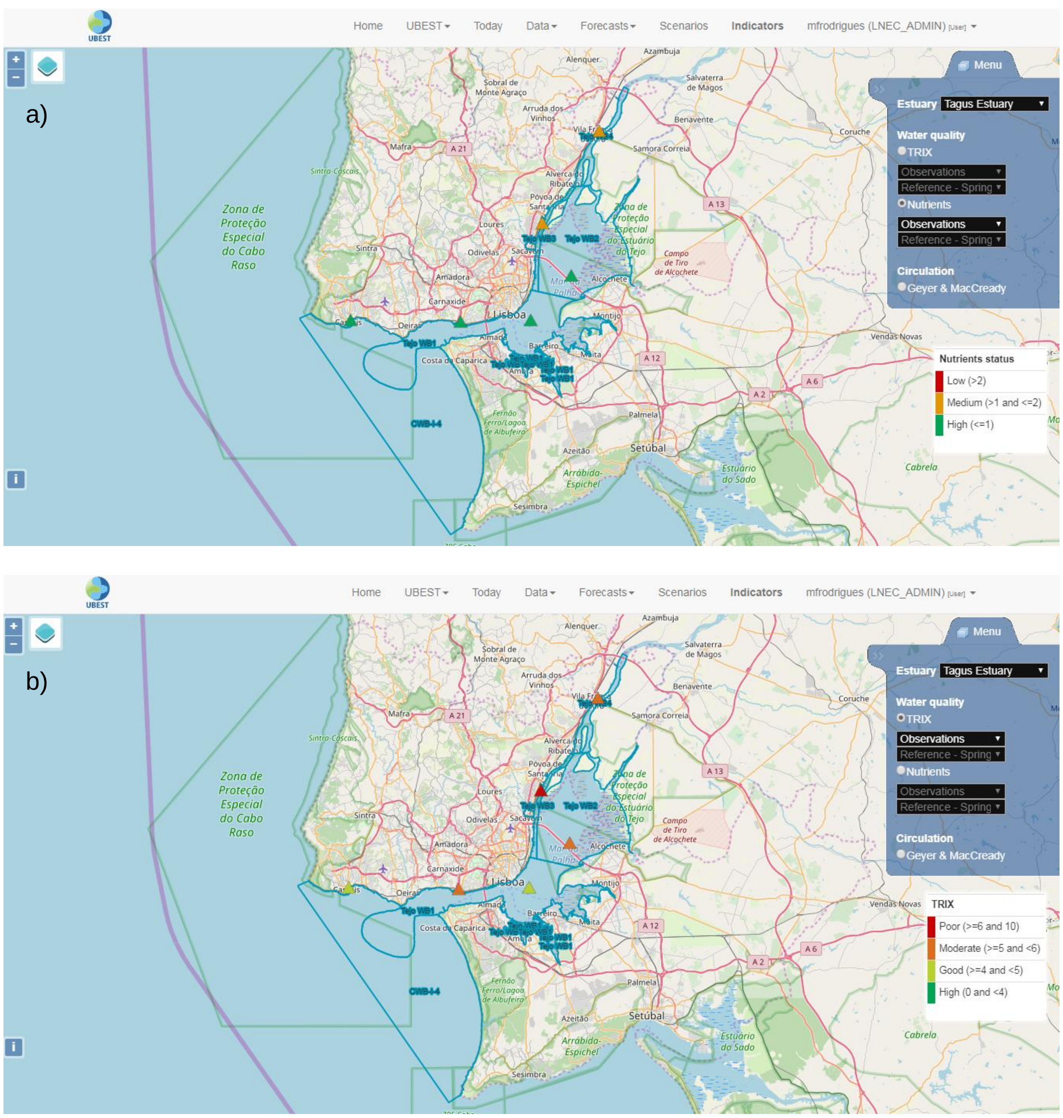

Figure 4. UBEST coastal observatory - 'Indicators' dashboard: a) nutrients chemical status and b) TRIX in the Tagus estuary based on 2018 field data. The indicators are depicted by the colors of the triangles.

Figure 5. UBEST coastal observatory - ‘Scenarios’ dashboard: mean ammonium concentrations in the Tagus estuary and for a user-selected point (blue circle within the estuary map) for different scenarios, a) reference scenario, b) sea level rise of 0.5 m and c) nitrogen and phosphorous increase of 50% at the riverine boundaries. The ammonium concentrations at the user selected point are presented on the right menu box.

- River flow decrease – this scenario considers a decrease of the river flow to 75% of the reference scenario. This scenario was based on the predictions for the average spring precipitation in 2071 ~ 2100 in the Lisbon Metropolitan Area considering RCP8.5, available at http://portaldoclima.pt/;
- Nutrients increase – this scenario considers an increase of 100% in the nutrients loads (ammonium, nitrate and phosphate) at the riverine boundaries;
- Nutrients decrease – this scenario considers a decrease of 50% in the nutrients loads (ammonium, nitrate and phosphate) at the riverine boundaries.

Simulations were performed only for the Spring season, when the primary productivity is highest, since the numerical models developed are very demanding computationally. The boundary conditions at the oceanic, riverine and surface boundaries of the reference scenario were established following a similar approach to Rodrigues et al. (2019). To set up the tide, statistics of the tidal amplitudes at Cascais (near the coastal boundary of the model) between 1991 and 2010 were computed (mean and standard deviation) using the tides from the regional model of Fortunato et al. (2016). The comparison of these values with their global mean and standard deviations indicates that the year 2001 is the most representative of average conditions. To define the atmospheric forcing a similar approach was used based on data from ERA-Interim (Dee et al., 2011, https://www.ecmwf.int/). An analysis of the statistics of the main representative variables (wind, air temperature, surface pressure and solar radiation) indicates that the year of 2001 is also the most representative of average conditions in the Tagus estuary. The river flow was established based on climatology estimated from data from the Almourol station. Salinity, temperature and other water quality tracers concentrations were established based on climatology.

3.1.3. Assessment of the Nutrients' Chemical Status

The Tagus estuary observatory provides information at different levels that allows users to assess the nutrients' chemical status and evolution in the Tagus estuary. Historical data, available since the 1980s, provide an overview of how nutrients' concentrations evolved over time in the estuary and suggests that high loads of nutrients have been reaching the estuary over time (Rodrigues et al., in review). The use of indicators, computed from 2018 data, suggests that the nutrient chemical status presents "High" quality in the downstream and middle areas of the estuary and "Medium" quality further upstream (Rodrigues et al., 2020; Figure 4). TRIX also presents a similar pattern: in the downstream area of the estuary the trophic status is "High" to "Moderate", while in the middle estuary and upstream is "Moderate" or "Poor" (Figure 4). Combining these data with an analysis of future scenarios provides further insight about the system response to changes, including CC or changes in the anthropogenic pressures, as exemplified below. The scenarios available for the Tagus estuary suggest that sea level rise slightly reduces the nutrients concentrations along the estuary (Figure 5). This reduction could be due to the growth of the tidal prism associated with the rise in sea level (Guerreiro et. al, 2015) and the resulting decrease of residence times. On the contrary, an increase in the nutrient inputs to the estuary from the rivers (e.g., due to increased loads from agriculture) has a more significant impact, with an increase of ammonium, nitrate and phosphate along the estuary. By quantifying the relative impact of different drivers, these data support decision-makers in the fine tuning of long-term management plans for this coastal system.

3.2. Daily Assessment of the Water Quality in the Ria Formosa

3.2.1. Study Area

The Ria Formosa is the most important ecosystem in the south coast of Portugal, and is classified as a Natural Park, a Ramsar wetland and a Natura 2000 site. It is a shallow barrier island system with about 100 km^2 that extends along 55 km in the west-east direction with a maximum width of 6 km in north-south direction. This coastal lagoon has a large intertidal area, which represents about 50% of the total area, mostly covered by sand, muddy sandflats and salt marshes. The Ria Formosa exhibits very dynamic and complex physiographic and morphologic features. The lagoon is delimited by five sandy barrier islands (Deserta, Culatra, Armona, Tavira and Cabanas) and two peninsulas (Ancão and Cacela) and connects to the Atlantic Ocean through six inlets. The inlets are linked by a complex network of interconnected channels, allowing the recirculation of water within the system and a permanent exchange with the adjacent ocean (Matias et al., 2008; Alcântara et al., 2012). The western sub-embayment (Ancão, Faro-Olhão and Armona inlets) is responsible for about 90% of the tidal prism of the lagoon (Jacob et al., 2013). The mean depth is 3.5 m, ranging from 6 to 13 m in the main channels and inlets (Falcão and Vale, 1990; Barbosa, 2010; Cravo et al., 2014). This lagoon is under the influence of semidiurnal tides, subject to a mesotidal regime, with a tidal range varying between 1.5 and 3.5 m (Jacob et al., 2013). Water renewal is high (between 50 ~ 75% daily; Tett et al., 2003) and the contribution of freshwater is negligible. The water characteristics of this lagoon are strongly regulated by the tidal exchanges and mixing with the coastal waters (Rosa et al., 2019a).

This ecosystem provides valuable resources for several economic activities in the region, namely tourism, aquaculture (e.g., major national producer of clams), shipping, fishing and salt production (50% of the national salt production) and it is used by several species as spawning and nursery areas. As the biological communities and the ecosystem services reflect the physicochemical environment conditions, it is essential to study the water quality status of this system. Variables such as temperature, salinity, pH, dissolved oxygen, chlorophyll a and nutrients are then key water quality parameters to take into account and to be measured in monitoring systems.

3.2.2. Model and Online Data Description

The numerical model of the Ria Formosa covers the entire lagoon and extends 30 ~ 35 km away from the coast. The hori-

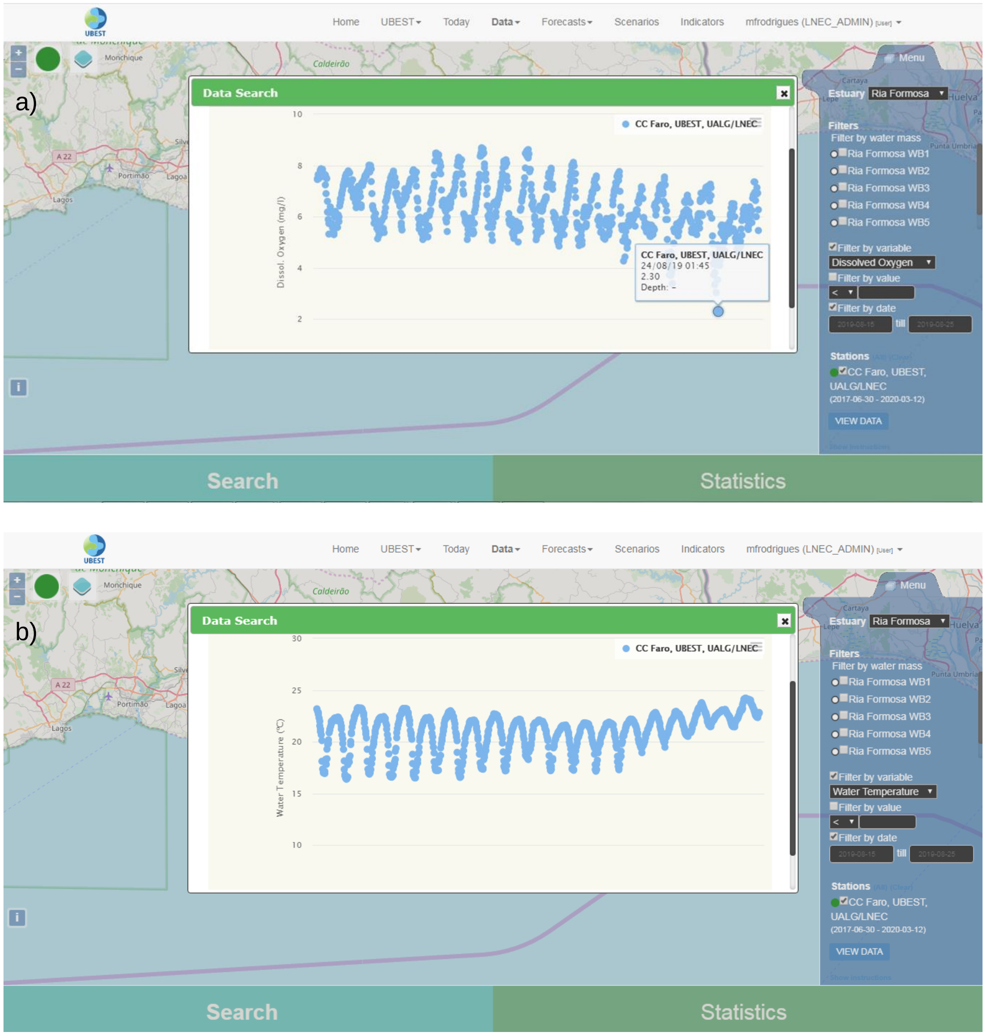

Figure 6. UBEST coastal observatory - 'Data' dashboard: a) dissolved oxygen and b) water temperature in the Ria Formosa between August 15 ~ 25, 2019.

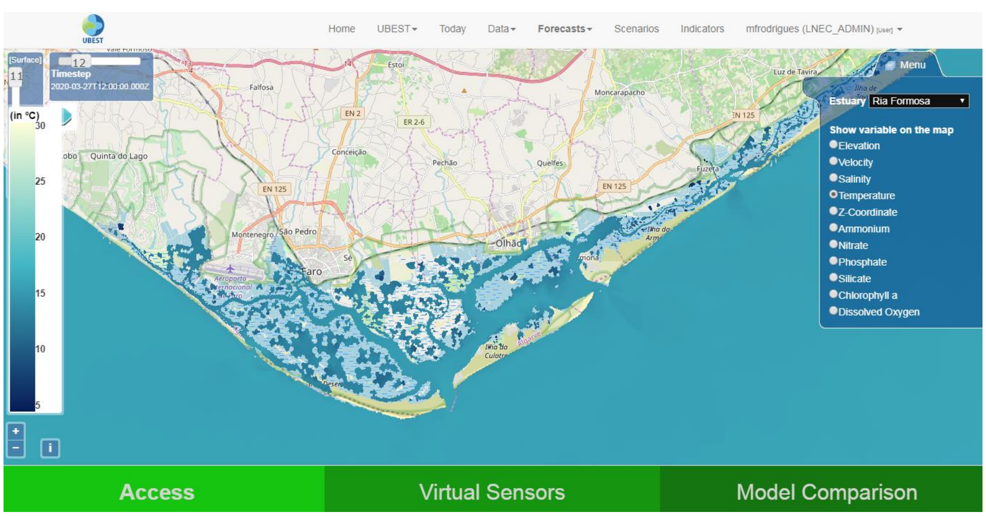

Figure 7. UBEST coastal observatory - 'Forecasts' dashboard: Forecast of the water temperature at the surface in the western sector of the Ria Formosa during low tide when extensive areas of the lagoon dry up.

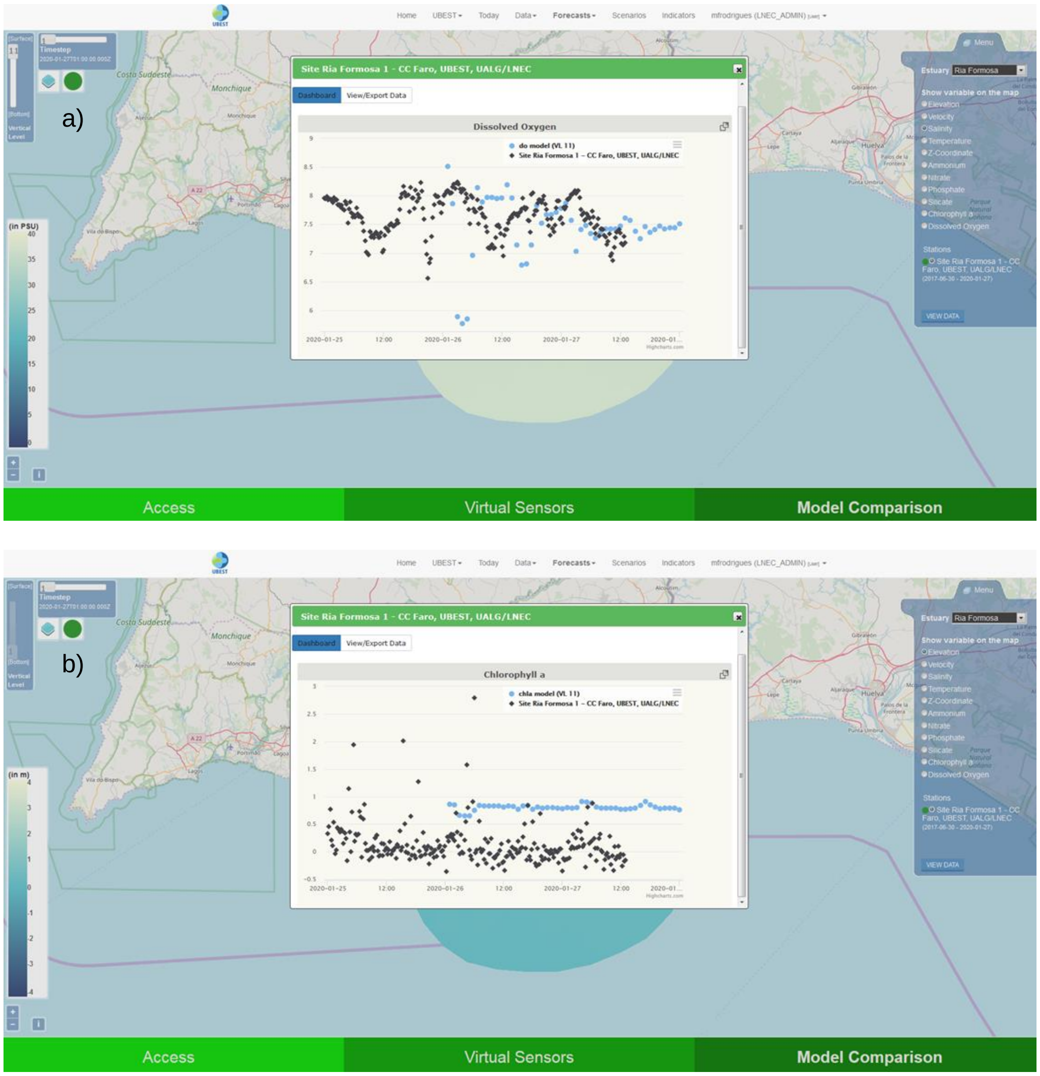

Figure 8. UBEST coastal observatory - ‘Forecasts’ dashboard: Comparison between real-time field data (black) and model forecasts (blue) of a) dissolved oxygen and b) chlorophyll a in the Ria Formosa.

zontal grid has about 98,000 nodes and a typical resolution that varies from 7 km near the coastal boundary to 10 m in the inner channels (Figure S6 in the supplementary materials). The vertical domain is discretized with a hybrid grid with 11 SZ levels (7 S levels in the upper 100 m, and 4 Z levels between 100 m and the maximum depth). The numerical model is forced by: i) tides, salinity, water temperature and water quality tracers’ concentrations at the ocean boundary; ii) river flows, salinity, water temperature and water quality tracers’ concentrations at the Gilão river boundary; and iii) atmospheric data at the surface. The model runs at about 1:8 of real time using 18 cores. Further details about the hydrodynamic model implementation can be found in Rosa et al. (2019b).

Similarly to the Tagus estuary numerical model, the model of the Ria Formosa was validated prior to its implementation in forecast mode by comparison with field data. In particular, physical, chemical and biological data from field campaigns performed specifically for the UBEST observatory were used (Cravo et al., 2017a, 2017b, 2017c). Some examples of the model and error measures results are presented in the Supplementary Material (Figures S7 and S8, and Table S2). Overall, the results show the model’s ability to represent the main spatial and temporal patterns of salinity, temperature, nutrients, chlorophyll a and dissolved oxygen observed in the Ria Formosa. The main differences arise from uncertainties in the boundary conditions, the existence of other point sources that were not considered in the model and processes related with the sediment-water exchanges that are absent in the model. Further details about the Ria Formosa model validation can be found in Rosa et al. (2019b).

As part of the Ria Formosa observatory, a real-time water quality station was installed within the inner part of Faro channel, in the vicinity of Port of Faro (37 °00′ 9.92″ N, 7 °55′ 16.28″ W), providing data for both the daily monitoring of the system and the continuous model validation. This station was equipped with an YSI EXO 2 multiparameter probe with sensors to measure water temperature and conductivity/salinity, pH, and optical sensors to measure dissolved oxygen, chlorophyll a and turbidity. The probe was set up to acquire data with a 15 min sampling interval and data were transferred hourly to the data repository.

3.2.3. Daily Monitoring of the Water Quality

The deployment of the Ria Formosa coastal observatory and, in particular, the access to real-time data and forecasts allows the user to capture the variability of the relevant water quality parameters at different temporal and spatial scales. One example of such parameters that is monitored is dissolved oxygen. Decreases of oxygen concentration associated with summer upwelling periods have been observed frequently (e.g., Figure 6). However, real-time data also show that events with low oxygen levels typical of hypoxia (2 mg/L) have been episodic and short-lived. The access to these monitoring data combined with the forecast results (Figure 7) provides useful information to support decision-makers in the adoption of timely response measures when needed. Moreover, real-time data are also used to assess the accuracy of the model predictions (Figure 8), providing further confidence in them and allowing the identification and correction of errors (Figure 8).

4. Conclusion

Considering the value of the ecosystem services provided by coastal systems, integrated observational systems are extremely important tools. These tools provide a valuable repository of data available in public web portals that can easily be accessed by several groups of interest. This allows not only the continuous surveillance of the system, crucial to advance knowledge about its natural variability, but also provides information essential to assessing the system's response to future scenarios. An informed data analysis used by decision-makers also supports management strategies' to protect and preserve these valuable systems.

Available infrastructures for data dissemination are typically global data repositories with sometimes embedded assessments on data quality (e.g., EMODNET or sea level data repository from the Hawaii university for sea level rise evaluation). They are not customized to address specific issues on a particular coastal system, neither do they allow for integrated analyses using multiple data sources. Their interfaces typically target facilitated (e.g., machine2machine) data access. On the contrary, observatories have a generic nature (materialized by a comprehensive data model and a generic forecast framework) but are customized for each system to take full advantage of the information available. They constitute the next step on data infrastructures, building from global repositories to local deployments and targeting local concerns of the end-users.

Coastal observatories are thus proposed and implemented herein as operational frameworks. The UBEST coastal observatory provides integrated data-model approaches to reach the continuous detailed ecological monitoring of the coastal systems and support short-term actions and long-term coastal management. Moreover, this innovative tool provides several flexible data-model services that can support both the continuous application of the European Water Framework Directive and emergency interventions in case of serious contamination events. While the type of information provided is not necessarily new, the speed at which it is made available can drastically improve the decision-making process. Observatories can foster the involvement of many stakeholders in the discussions and encourage the exploration of alternative scenarios, ultimately leading to better and faster decisions. Similarly to the facilitated procedure to address decision-makers concerns, these tools also help researchers to build knowledge and address scientific questions through the exploitation of the observatories and their information services. The UBEST observatory provides a valuable source of information to fill-in the voids from data stations and the surface-only data from remote sensing, and integrates in a single interface data from the hydrodynamics and biogeochemical simulations, providing the capacity to use them seamlessly to compute indicators and understand long-term trends.

The concept of observatory proposed herein was implemented through a generic IT framework, where a careful design and implementation strategy allows the UBEST observatory portal to be easily deployed in the future to other coastal systems. Besides its general applicability, UBEST provides several services to understand biogeochemical evolution in a given estuary, providing a one-stop-shop for all relevant data and models, and allowing the easy integration of new sensors and indicators. The combined use of all information is novel and provides the ground for new studies to be performed in other systems, taking advantage simultaneously of historical and real-time data. There are many platforms available in the literature that address some of these assets but none addresses them all. The availability of a customizable tool for any coastal system, such as the UBEST observatory, also paves the way for generalized analyses of climate change impacts in estuaries' biogeochemistry worldwide, a better understanding of global trends and interactions and searches for common solutions. Through this integrated procedure, the classification of estuaries regarding their biogeochemical dynamics can be achieved and the knowledge be extrapolated from highly monitored systems to estuaries with little or no data.

The challenge for a broad application of UBEST concepts relies on two aspects: 1) the availability of computational resources for the daily water quality predictions at the required spatial scale, computation of the associated indicators and access to data, and 2) the capacity for building up the team of coastal scientists and computer science experts to adapt UBEST for their system of interest. The former can be addressed through integration with high-performance or distributed computing environments such as the European Open Science Cloud (EOSC), requiring new strategies for high model efficiency, for instance linking CPU and GPU paradigms, as well as distributed and HPC computing. The latter may prove quite complex to achieve. A potential solution may be the development of a UBEST e-service, where any user with a capacity to build a computational grid and enough knowledge of ecological processes can interact with a web on-demand platform to build his/her own system. This concept, denoted as OPENCoastS, has already been demonstrated for coastal hydrodynamic predictions (Oliveira et al., 2020) and is in operation since 2018 supported by the EOSC-hub computational infrastructure. Besides the challenges of adapting OPENCoastS to biogeochemical predictions, the data integration and data/model services needed for a generic, on-demand, UBEST observatory are far from trivial.

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