Deliverable report - RiOMar Project

Task 3.1	- Due date: 03/2024 - Date of report: 03/2024	Deliverable number and title: **D3.1 - Protocol for numerical simulation experiments**	Person in charge LOPS (G. Charria)

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Abstract:
The RiOMar project aims at improving our understanding of the evolution of coastal regions under the influence of main rivers along French coasts during the 21rst century. At the interface between academic research and environmental managers, we need to evaluate the future evolution of those vulnerable ecosystems to define possible solutions to adapt our actions to climate change impacts.
Such a project needs to design numerical experiments to feed a digital twin of the coastal ocean in agreement with the targeted coastal ocean regions and associated processes (in terms of resolution, forcings, solved processes).
The present deliverable sets out in detail numerical models and planned experiments. Following obtained results and future discussions with environmental managers, those experiments will be adapted to reach project objectives.

Deliverable report :

1. Introduction

The RiOMar Project aims at defining and building, with environmental managers, an original integrated approach combining augmented observatories, innovative digital tools and model simulations to anticipate the future of coastal ecosystems under the influence of rivers during the 21st century. One of the core components of the project is based on the development of numerical simulation experiments based on existing ocean models implemented to simulate RiOMar regions in the Mediterranean Sea, the Bay of Biscay and the English Channel. Numerical simulation experiments in those regions need to be designed to reproduce ocean processes including the complex hydrodynamics and sediment dynamics, the pelagic and benthic biogeochemistry, the productivity of the first levels of marine food webs. Those experiments will be the backbone of the Coastal Ocean Digital Twin proposed in the project.
Several modeling strategies can be adopted for such experiments generally combined with the support of large-scale computing capacities.
The present deliverable will detail the protocol used for numerical simulation experiments in RiOMar. The ocean model features will be detailed as well as the adopted strategies for implementing climate simulations in coastal oceans under river influence.

2. Model description

To simulate coastal ocean dynamics and coupled processes between Developed model configurations are based on four compartments

- Hydrodynamics
  - SYMPHONIE

To simulate the dynamics of the Mediterranean sea we use the 3-D ocean circulation model SYMPHONIE (Marsaleix et al., 2008, 2019). It is based on the Navier-Stokes primitive equations solved on an Arakawa curvilinear C-grid under the hydrostatic and Boussinesq approximations. The model makes use of an energy conserving finite difference method described by Marsaleix et al. (2008), a forward-backward time stepping scheme, a Jacobian pressure gradient scheme (Marsaleix et al., 2009), the equation of state of Jackett et al. (2006), and the K-epsilon turbulence scheme with the implementation described in Costa et al (2017). Horizontal advection and diffusion of tracers are computed using the QUICKEST scheme (Leonard, 1979) and vertical advection using a centered scheme. Horizontal advection and diffusion of momentum are each computed with a fourth order centered biharmonic scheme as in Damien et al (2017). The biharmonic viscosity of momentum is calculated according to a Smagorinsky-like formulation derived from Griffies and Hallberg (2000). The lateral open boundary conditions, based on radiation conditions combined with nudging conditions, are described in Marsaleix et al. (2006) and Toublanc et al. (2018).

The VQS (vanishing quasi-sigma) vertical coordinate described in Estournel et al, (2021) is used to avoid an excess of vertical levels in very shallow areas while maintaining an accurate description of the bathymetry and reducing the truncation errors associated with the sigma coordinate (Siddorn et Furner, 2013).

The implementation of the tide, described in Pairaud et al (2008, 2010), consists on the one hand of the amplitude and phase of the tide introduced at the open lateral boundaries and on the other hand of the astronomical plus loading and self-attraction potentials. The 9 main harmonics of the tide are considered, the forcing fields being provided by the 2014 release of the FES global tidal model (Lyard et al, 2021). On the continental shelves, the turbulence generated by the friction of the tidal currents on the bottom is generally significant. Near the bottom the temperature and salinity stratification is in principle homogenized over a layer that can be up to several tens of meters high depending on the strength of the tide. OGCM fields provide boundary conditions for temperature, salinity, surface elevation and currents associated with non-tidal processes. Because the tide is not taken into account in the OGCM simulation, the stratification is insufficiently mixed near the bottom. As the errors induced on T and S are potentially important, we make a modification to the OGCM T,S fields before introducing them at the open boundaries of our model (Nguyen-Duy et al., 2021). This modification consists in homogenizing T and S near the bottom, over a thickness deduced from the expected theoretical height of the tidally induced turbulent bottom layer. This height is estimated from the friction velocity associated with the tidal current, i.e. $D = 0.1u^{*}/f$ (Csanady, 1982) where f is the Coriolis parameter and the friction velocity, u^{*}, is calculated from the tidal harmonics of the depth-averaged current provided by FES, and a drag coefficient of 10^{-3}.

The quadratic Von-Karman law (logarithmic law) is used for bottom friction with a bottom roughness z0 = 1 mm. The atmospheric fluxes are calculated for the RiOMar simulations using the ECUME parameterization (Roehrig et al., 2020).

- CROCO (Coastal and Regional Ocean COmmunity model)

To simulate the hydrodynamics in the Bay of Biscay and the English Channel, the Coastal and Regional Ocean COmmunity model (CROCO - https://www.croco-ocean.org - Ayouche *et al.*, 2021; Auclair *et al.*, 2022) is implemented. CROCO (built on ROMS model - Shchepetkin and McWilliams, 2005) is a split-explicit, free-surface, hydrostatic, primitive equation ocean model. The model equations are discretized on an Arakawa C-Grid and use sigma coordinates for vertical dimension and orthogonal curvilinear coordinates for horizontal dimension. Vertical layers are stretched at the surface and at the bottom with $\theta s = 6$, $\theta b = 4$ and hmin = 15m.
The horizontal advection of momentum and tracers is performed with the split and rotated 3rd-order upstream biased advection scheme (RSUP3 - Marchesiello et al., 2009) and the vertical advection of momentum and tracers is performed with a 4th-order compact advection scheme (SPLINES). The model turbulent closure scheme is based on a Generic Length Scale model corresponding to a k-epsilon turbulence scheme (Jones and Launder, 1972; Umlauf and Burchard, 2003). The quadratic Von-Karman law (logarithmic law) is used for bottom friction with a bottom roughness z0 = 10 mm.
The tidal sea surface elevation and currents with 15 harmonic constituents are imposed along the boundaries using the FES2014 ocean tide atlas (Lyard et al., 2021).

For all simulations covering a region with a strong semi-diurnal tidal signal, hourly outputs are written and saved during simulations. Due to the large amount of data to write (3.3To per simulated year), model NetCDF4 outputs are created using the XIOS 3.0 (https ://forge.ipsl.jussieu.fr/ioserver) library. This library allows dedicating cores only for reading and writing tasks. In our computing infrastructure, each node is based on 28 cores with 27 cores dedicated to model equations and 1 core dedicated to XIOS server.

- Sediment dynamics
    - MUSTANG

The sediment dynamics is modeled by the MUSTANG (MUd and Sand TrANsport modelliNG - Le Hir et al., 2011; Grasso et al., 2015; Mengual et al., 2017; Grasso et al., 2021) sediment module. This code allows introducing sediment behavior in the water column and sediment bed evolution for cohesive and non-cohesive mixtures. In the water column, the sediment is transported based on solved advection/diffusion equations as a passive tracer with a settling velocity accounting for flocculation processes for different classes of particles in the water column. Particles from sediment bed are advected following a critical bed stress and remain close to the bottom.
MUSTANG is a multi-layer model (layers with variable thickness ranging from 1 µm to 5 mm) including gravel, sand and mud classes. Gravels are advected only in bedload (no suspension). Sands can be advected by both types. Muds are advected only in suspension (no bedload).

For RiOMar coupled simulations in the Mediterranean Sea, the Bay of Biscay and the English Channel, the MUSTANG model will be used to simulate sediment dynamics. Based on our knowledge on the sediment nature and dynamics in those regions, MUSTANG configuration will be adapted in both configurations (e.g. number of layers, sediment classes, initial conditions).

- Biogeochemistry
    - ECO3M-S

The biogeochemistry of the Mediterranean Sea is simulated using the ECO3M-S model (Ulses et al., 2016). The model describes the cycles of carbon, nitrogen, phosphorus and silicate. It includes three phytoplankton and three zooplankton groups as well as a bacteria compartment. The phytoplankton component is based on the model developed by Baklouti et al. (2006) and the heterotroph component on the model on Anderson and Pondaven (2003). It was recently expanded to describe dissolved oxygen and inorganic carbon dynamics (Ulses et al., 2021; 2023). It is coupled with a seabed vertically integrated diagenesis model based on Soetaert et al. (2000). A detailed description and an assessment on the Gulf of Lion shelf are given by Auger et al. (2011) which analyzed the mechanisms and Many et al. (2021).
In the framework of the current project, we will test different levels of complexity of the coupling between the water column models and the diagenesis model: (i) less computational demanding vertically integrated model with meta-modelling to set the bulk parameters (Soetaert et al., 2000; 2001), (ii) vertically resolved model based on OMEXDIA and FESDIA (Soetaert et al., 1996; Nmor et al., 2022) models, and (iii) coupling with sediment transport model to take into account deposition/resuspension events (Capet et al., 2016).
The biogeochemical model is forced offline by the daily outputs (current velocities, turbulent diffusion coefficient, temperature and salinity) of the SYMPHONIE model.

    - BLOOM (BiogeochemicaL cOastal Ocean Model)

The biogeochemistry for the Bay of Biscay and the English Channel is simulated using the BLOOM model (BiogeochemicaL cOastal Ocean Model - Plus et al., 2021) derived from the ECO-MARS model (Cugier et al., 2005; Ménesguen et al., 2019) and adding major processes of early diagenesis. The BLOOM model is built on three phytoplankton groups (microphytoplankton - diatoms, dinoflagellates and pico-nano-phytoplankton), the micro- and mezo-zooplankton, nutrients, detrital material and exchanges at the water-sediment interface and inside the sediment compartment. Nitrogen, phosphorus, and silica cycles are modeled considering four nutrients: nitrate, ammonium, soluble reactive phosphorus, and silicic acid (sorption/desorption of phosphate on suspended sediment and precipitation/dissolution of phosphate with iron processes are also included).
The variables and processes added to BLOOM were chosen by selecting the simplest solution, in order to maintain a model that can be used to simulate realistic 3D configurations at fine resolutions. For nitrogen and phosphorus cycles, variables are decomposed in a labile and refractory fraction. Whole equations for different cycles are detailed in Plus et al., 2021.
In the framework of the project, the biogeochemical BLOOM model will be first coupled online with the hydrodynamical and the sediment transport modeling hindcast simulations. An offline approach forced by hourly outputs is planned to be implemented for exploring sensitivity experiments to biogeochemical forcings sensitive to river runoffs in future scenarios.

- Contaminants

A preliminary exploration of the dynamics of various contaminants, for which sorption coefficients for dissolved and particulate carbon are well-documented, can be formulated following the biogeochemical dynamics phase.

3. Model configurations

Based on those models, two main configurations for hydrodynamical models have been developed for the western Mediterranean Sea (SYMPHONIE/BlueLion - Figure 1) and the Bay of Biscay / English Channel (CROCO/GAMAR configuration - Figure 2).

RiOMar model configurations are defined by the following features:

Region	**North-West Mediterranean**	**Bay of Biscay / English Channel**
Configuration	**SYMPHONIE / BlueLion**	**CROCO / GAMAR**
Domain	33°N - 44.5°N / 1.2°W - 16.3°E with a bipolar grid	43.3°N - 50.9°N / 8°W - 1.7°E
Horizontal resolution	340m - 4.5km (minimum in the NW Mediterranean)	1km
Grid size	1230 x 1308 x 50	727 x 838 x 40
Vertical coordinates	VQS (vanishing quasi-sigma)	Generalized sigma coordinates
Rivers	77	23
Tidal forcing	FES2014 - Lyard et al., 2021	FES2014 - Lyard et al., 2021

As an example, the BlueLion configuration is currently running on 1535 cores. About 20 hours real time is needed for a one year simulation on the BELENOS computer of Meteo-France. For the GAMAR configuration, the model is running on 1740 cores. About 12 hours real time is needed for a one year simulation on the Joliot-Curie/Irene Rome computer at CEA (French Alternative Energies and Atomic Energy Commission).

Bathymetry has been defined from combinations of existing products. For SYMPHONIE, the bathymetry is built from the GEBCO database, the Digital Terrain Model Gulf of Lion - Azur Coast from SHOM, the Litto3D Languedoc Roussillon database in the littoral band and a data base around the Rhone mouth based on the merging of two recent bathymetric cruises from Europe and Haliotis vessels. For CROCO/GAMAR, a Digital Terrain Model has been built from 100m resolution from the HOMONIM bathymetry from the Shom (https://data.shom.fr) until 6°W and then 115m resolution Emodnet bathymetry for regions E3 and E4 (https://portal.emodnet-bathymetry.eu) is considered. The different Digital Terrain Model are merged on a 200 m resolution grid using BMGtools software (Theetten *et al.*, 2014). The bathymetry was then smoothed to limit pressure gradient errors. The minimum depth is 8 m (for example in estuaries) and the maximum depth at the western boundary is ~ 4 350 m.

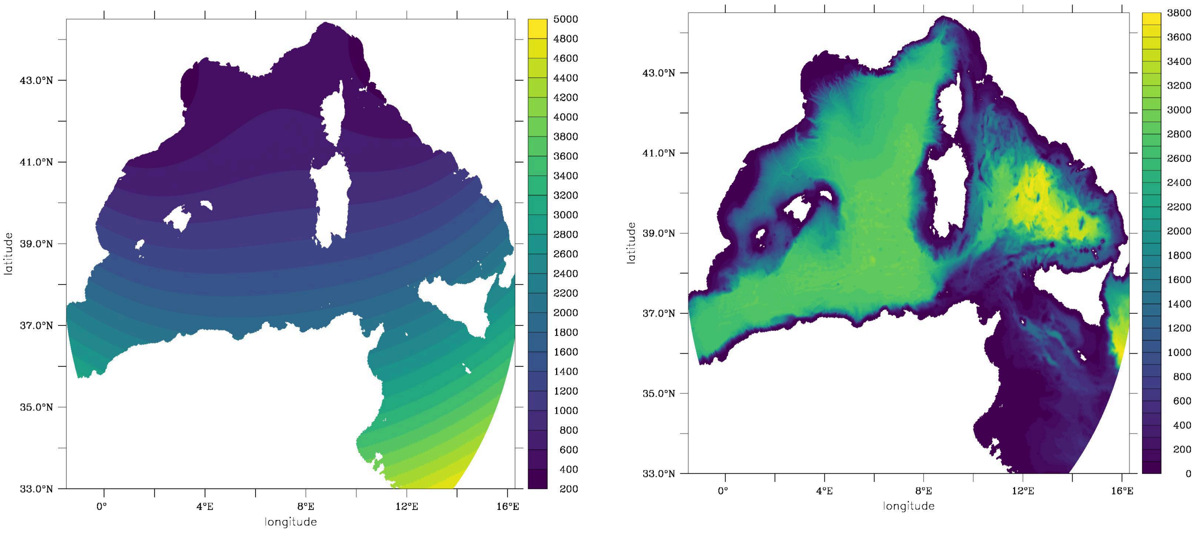

Figure 1 - BlueLion configuration of the SYMPHONIE model: variable horizontal grid resolution in meter (left) and bathymetry (right).

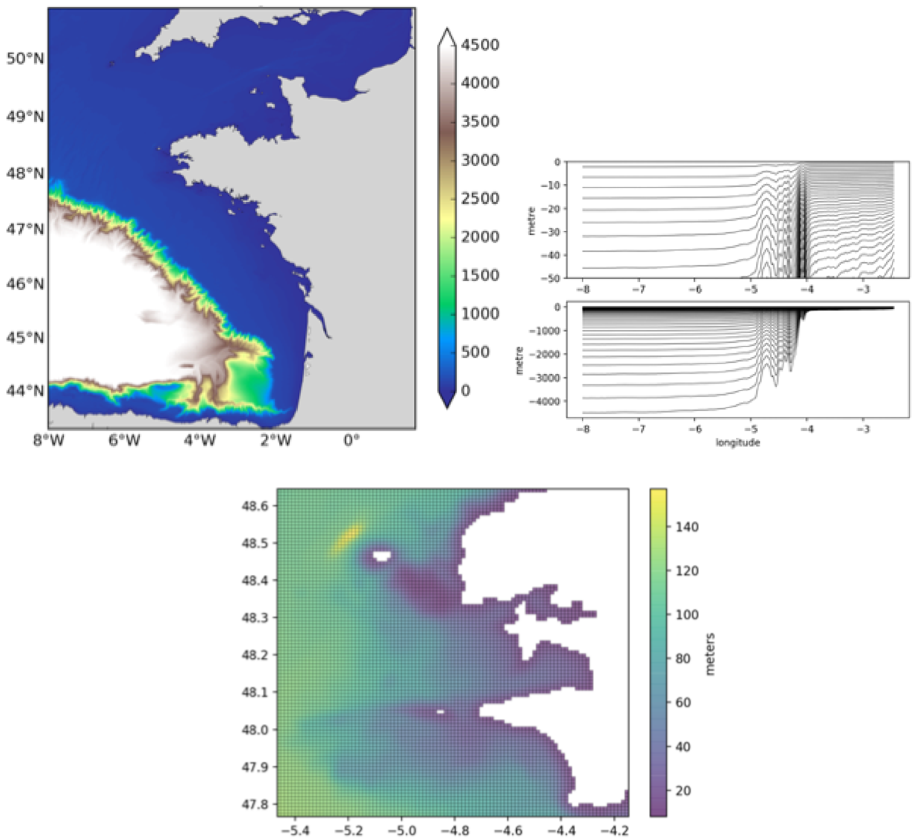

Figure 2 - (a) CROCO/GAMAR model domain and bathymetry and (b) East-West vertical sections at 46°N of the 40 sigma vertical levels over 50 m depth (top) and the whole water column (bottom) (c) 1 km grid zoom over the Iroise sea

4. Simulation strategy / scenarios

To explore the coastal ocean dynamics under river influence, several numerical experiments have been designed and will be implemented during the RiOMar project. Combining **needs** (*e.g.* high resolution simulation to model coastal processes, long-time period to study the 21st century) and **constraints** (*e.g.* strong interannual variability to consider in future scenarios, expensive computing simulations in terms of time and storage capacities), a numeral experiment strategy has been designed based on 4 main "reference" simulations (Figure 3).

Those 4 "reference" simulations are divided in:

- (1) 20-25 year hindcast "real Ocean"
- (2) 25 year hindcast "climate"
- (3) 20 year scenario from 2030 to 2050
- (4) 20 year scenario from 2080 to 2100

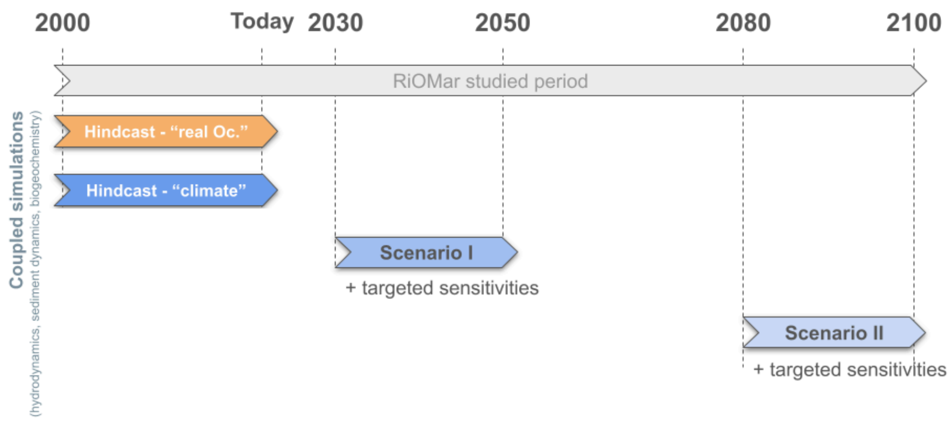

Figure 3 - Overview of planned numerical experiments in RiOMar

(1) 20-25 year hindcast "real Ocean"

This simulation is built, based on the state of the art, on the best forcing combination to reproduce long-term variability of the coastal ocean during the last two decades. Those experiments are then based on reanalysis for atmospheric and open boundary conditions[1] and on real observations for river discharge. After the validation process, those simulations will be key experiments to understand processes driving interannual variability simulated in RiOMar regions. They will be jointly analyzed with collected *in situ* observations in the project. They will also be used for building advanced products based on Artificial Intelligence algorithms.

Linked with addressed questions in regional work packages, nested higher resolution simulations could be implemented to solve local physical or biogeochemical processes. At this stage of the project, such nested approaches are under consideration in Pertuis Sea and in English Channel.

[1] For example in CROCO/GAMAR "real Ocean" simulation, atmospheric forcing are based on ERA5 reanalysis (Hersbach *et al.*, 2020) and initial open boundary conditions are based on GLORYS12V1 reanalysis, a CMEMS global product (1/12° horizontal resolution, 50 vertical levels - https://doi.org/10.48670/moi-00021).

(2) 25 year hindcast “climate”

Simulating the same past and ongoing time periods as the hindcast “real Ocean”, the simulation called hindcast “climate” will be the key experiment to evaluate how coastal models in RiOMar region can be nested in climate simulations. Indeed, this simulation will aim to reproduce the last two decades using forcings from large scale coupled land-ocean-atmosphere climate experiments that will be used for future scenarios. This simulation will allow developing and/or refining our modeling techniques to force a coastal model with climate coupled large scale numerical experiments. Several issues such as gaps in spatial resolution between large scale ocean model and our coastal model, bias in coupled simulations (e.g. river discharge, mean temperature) will be addressed in this experiment. Developed techniques for this experiment will be used for future scenarios.

This experiment will also allow evaluating uncertainties we can meet with future scenarios forced by climate models. Indeed, this experiment will allow quantifying the coastal ocean variability we will be able to reproduce in future experiments.

The initial and open boundary conditions and the atmospheric forcing will be given by the 6 *th* generation of the CNRM RCSM (CNRM-RCSM6), regional climate system model (atmosphere, ocean, land surface hydrology) developed at CNRM (Météo-France) over the Mediterranean CORDEX domain (Med-CORDEX) but also covering the Bay of Biscay / English Channel region. Those coupled simulations are based on the NEMO model at 1/12° for the ocean, the Aladin-Climat model at 12 km for the atmosphere and the ISBA-CTRIP land surface hydrology model. A first run of the BlueLion configuration has been forced with this configuration over the period 2000-2019. The biogeochemical model will be forced by the same biogeochemical model implemented at the Mediterranean scale and forced by the hydrodynamic and atmospheric CNRM-RCSM6 model. For the GAMAR configuration, ongoing analyses are exploring forcing features (for atmosphere and rivers) compared with reanalysis over hindcast period.

(3) 20 year scenario from 2030 to 2050

This mid-term experiment is one of the main aims of the project because it represents key time scales for environment managers. Indeed, this experiment is designed to simulate RiOMar region variability from 2030 to 2050. This simulation will be based on developments performed for the hindcast “climate” simulation. As it will reproduce future variability, our validation process will be adapted (no reference observations).

Same as for the hindcast climate, we plan to use the SSP3-7.0 scenario currently planned at CNRM[2]. The scenarios of river biogeochemical forcing will be co-constructed with the managers.

(4) 20 year scenario from 2080 to 2100

This long-term experiment for the period 2080-2100 will give an overview of coastal ocean variability at the end of the century. Following the same settings as the scenario from 2030 to 2050, simulations will benefit our experience on previous experiments and the same strategy could be applied.

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[2] For development purposes in the meantime and in case of delays in SSP3-7-0 simulations, RCP8.5 scenario of the CNRM-RCSM6 will be used.

Same as for the hindcast climate, a first run SYMPHONIE-BlueLion in the Mediterranean Sea forced by the scenario RCP8.5 of the CNRM-RCSM6 has been performed over the period 2080-2099. In the frame of RiOMar, we expect to use the SSP3-7.0 scenario currently planned at CNRM.
A similar strategy is planned for CROCO-GAMAR configuration in the Bay of Biscay and English Channel.

To perform such 4 reference simulations, several added numerical experiments are needed. First, configurations need to be designed, calibrated and validated for studied regions. Then, we need to compute intermediate simulations not including the whole compartments (*e.g.* hydrodynamical hindcasts are first produced). Finally, due to the cost of simulation, we need to focus on one climate scenario. However, we know that such a scenario is subject to large uncertainties. During the project, we will then investigate possibilities to perform sensitivity experiments (at least on biogeochemical compartment to evaluate impacts of changes from river nutrient discharge in coastal ocean).

5. Data storage and diffusion

RiOMar numerical experiments will represent a large amount of data (several tens of terabytes) initially stored in Météo-France (Belenos computer) and CEA (French Petascale machine Curie in Computing Center for Research and Technology) supercomputers. First analyses will be performed directly on those computers but RiOMar project aims to give access to this information. Two levels of diffusion are planned in the project:
- The diffusion of **raw simulated fields** using optimized extracting tools (based on most recent advanced Python parallel computing libraries as Xarray and Dask). Those fields will be extracted and distributed for given subregions (and depths) and targeted time periods through compressed binary files (netCDF format). The processing and the analyses of such fields will need research center computing facilities (as local computing centers - *e.g.* Datarmor supercomputer from Ifremer) and advanced skills in operating such datasets.
- The second level of diffusion will be addressed to a wider range audience, including environmental managers. For this purpose, **processed simulated fields** will be published (on dedicated web services and portals). Those datasets will either be extracted simulations for direct use or applications (as Sea Surface Temperature or Salinity averages) or advanced products (data or figures) based on RiOMar dedicated processing (*e.g.* area influence of freshwater in coastal ocean, trends along simulated periods). Those products will be designed in the project with regional Work Packages and environment managers.

The strategy behind data storage and diffusion will, in any cases, be to give an easy and open access to numerical experiment data produced in the RiOMar project.

Publications, thesis, master internship (associated to the deliverable):

PhD Thesis (2023-2026) - Maud Martinez Almoyna Carlhand

ECOCIFS - Evolution of River-influenced Coastal Ecosystems in the Bay of Biscay and English Channel during the 21st Century

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