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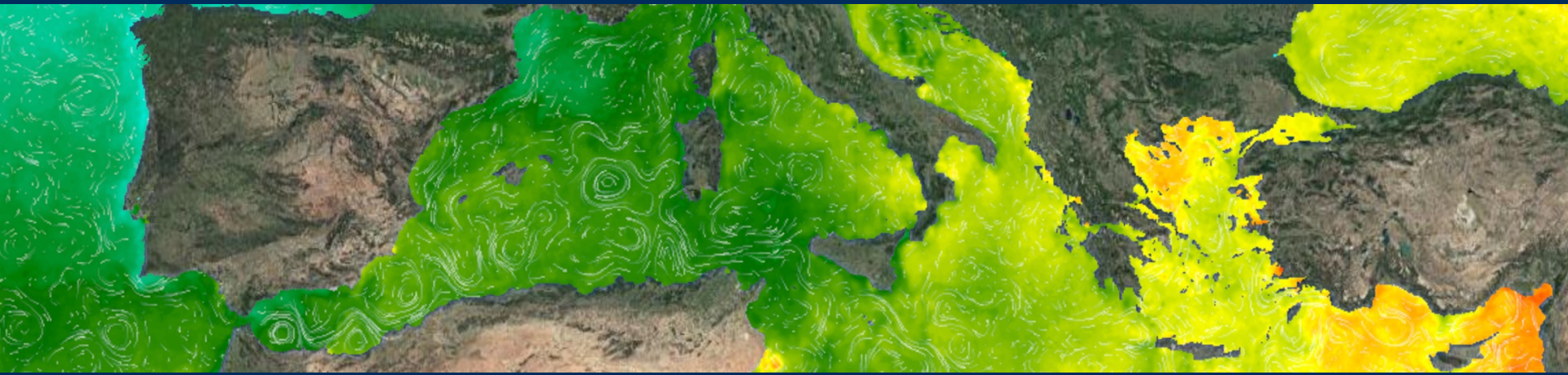

4DMED-sea

A data-driven approach to study the interactions between ocean dynamics and the marine ecosystem in the Mediterranean: the 4DMED-Sea project

Bruno Buongiorno Nardelli (on behalf of the 4DMED-Sea team)

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The team

core partners

extended team

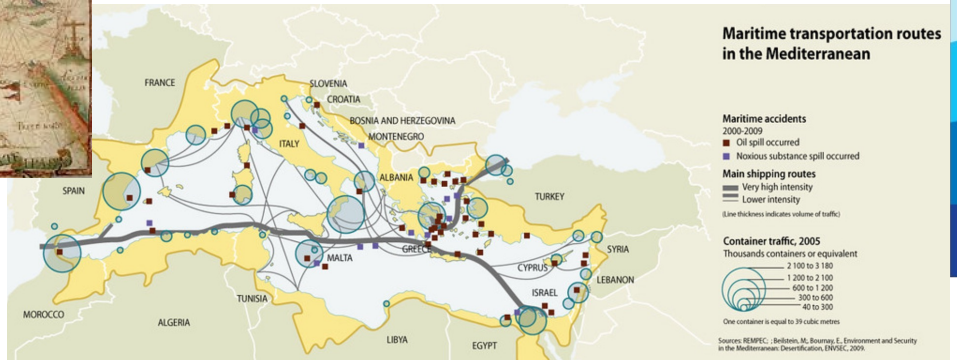
4DMED-Sea

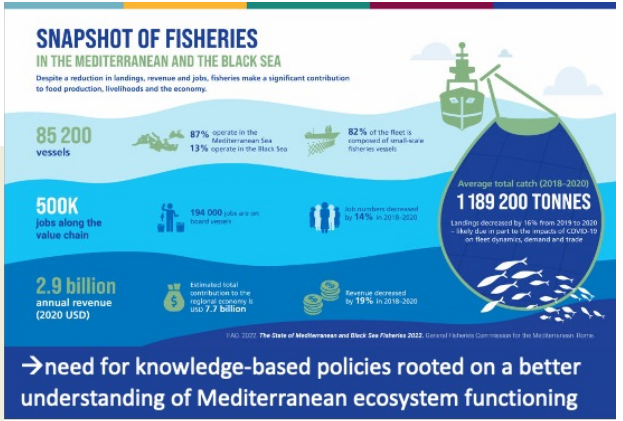
Bruno Buongiorno Nardelli[1], Claudia Cesarini[2], Vincent Rossi[3], Marina Levy[4], Nathalie Verbrugge[5], Ismael Hernandez-Carrasco[6], Astrid Bracher[7], Federico Falcini[1], Alain Arnaud[8], Simone Colella[1], Daniele Iudicone[1], Emanuele Organelli[1], Michela Sammartino[1], Rosalia Santoleri[1], Leo Berline[3], David Nerini[3], Francesco D'Ovidio[4], Roy El Hourany[4], Clement Haeck[4], Sandrine Mulet[5], Eric Greiner[5], Yannice Faugere[5], Marie Isabelle Pujol[5], Anaelle Treboutte[5], Maxime Ballarotta[5], Jeremy Augot[5], Ananda Pascual[6], Hongyan Xi[7], Marina Tonani[8], Ronan Fablet[9], Clement Ubelmann[10]

[1]Consiglio Nazionale delle Ricerche - Istituto di Scienze Marine, Italy; [2]Innuere Consulting, Italy; [3]Aix-Marseille Université, France; [4]Centre National de la Recherche Scientifique, France; [5]Collecte Localisation Satellites, France; [6]Consejo Superior de Investigaciones Científicas, Spain; [7]Alfred Wegener Institute, Germany; [8]Mercator Ocean International, France; [9]IMT Atlantique, France; [10]Datlas, France

The context

The Mediterranean Sea supports large and complex human socio-economic systems





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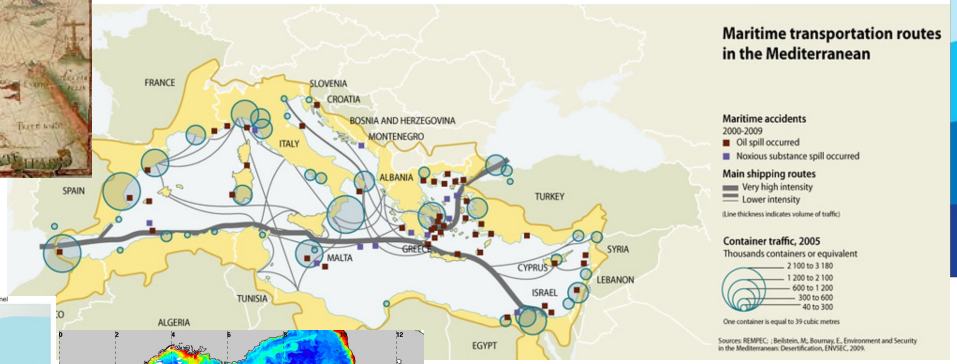
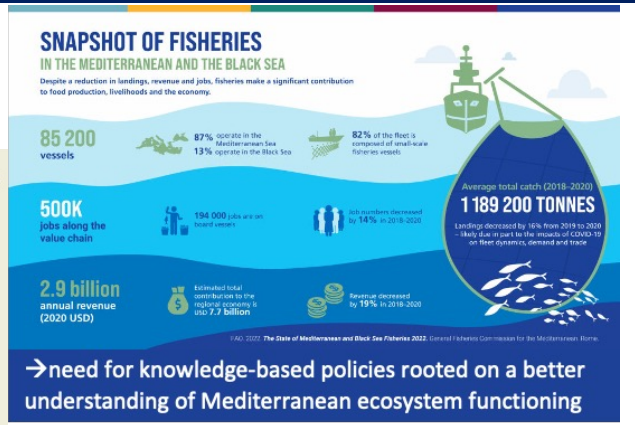
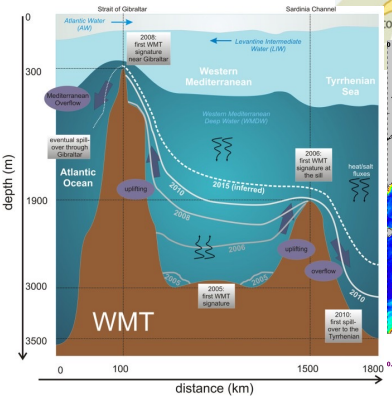
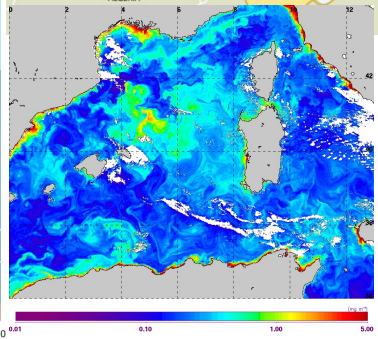
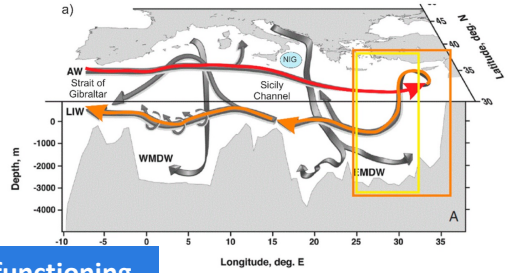




→need for knowledge-based policies rooted on a better understanding of Mediterranean ecosystem functioning



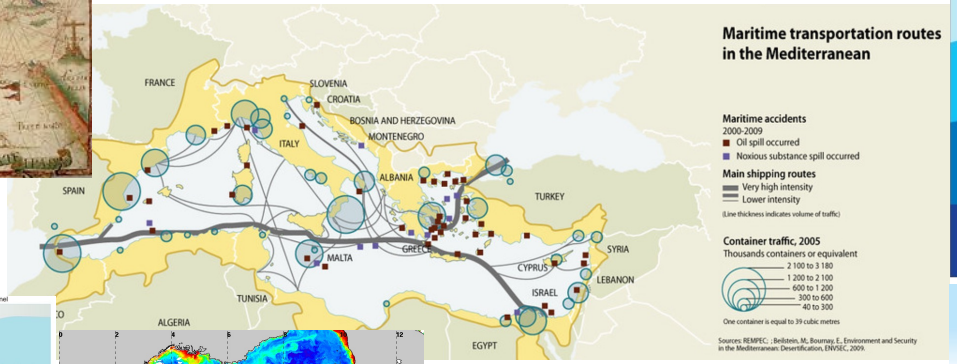


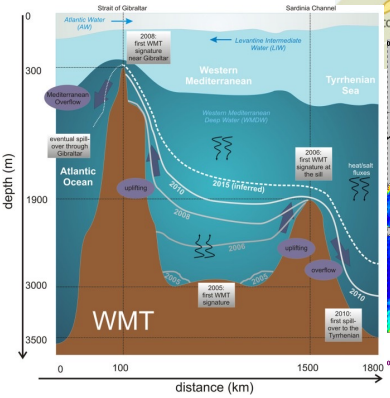


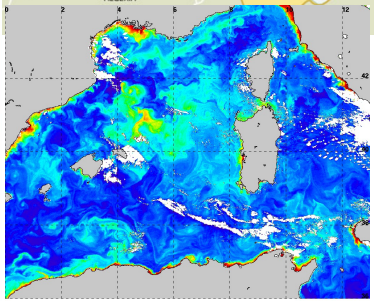
The Mediterranean Sea dynamics and marine ecosystem functioning are modulated by processes occurring at very different scales

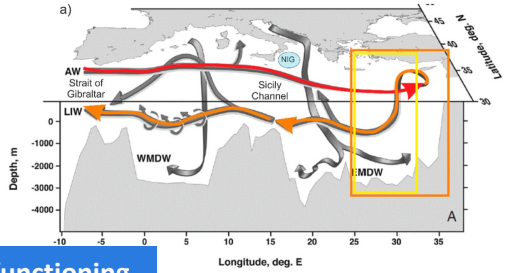
The context

The Mediterranean Sea supports large and complex human socio-economic systems

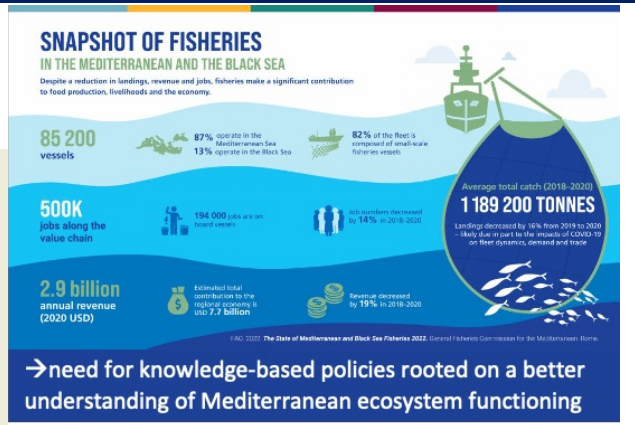




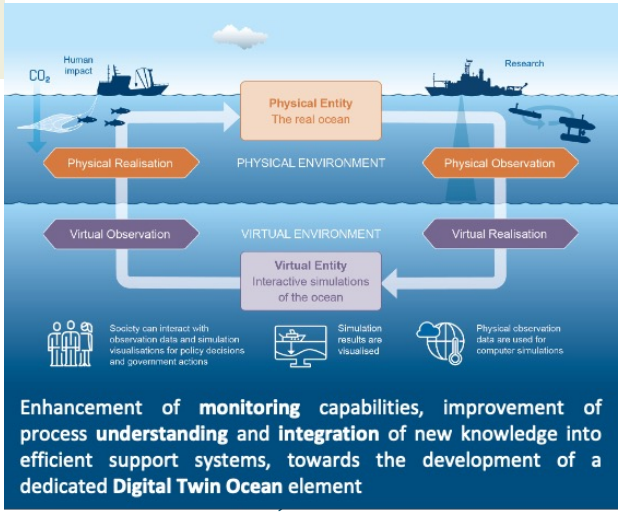




The Mediterranean Sea dynamics and marine ecosystem functioning are modulated by processes occurring at very different scales



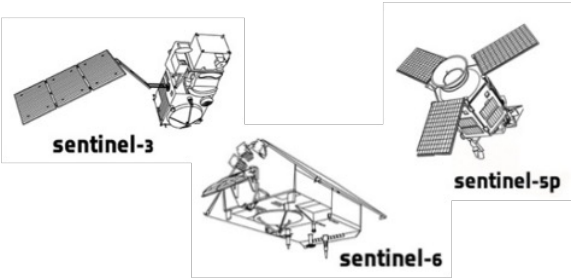
→need for knowledge-based policies rooted on a better understanding of Mediterranean ecosystem functioning

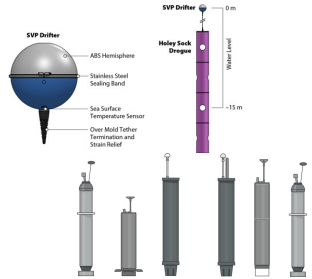


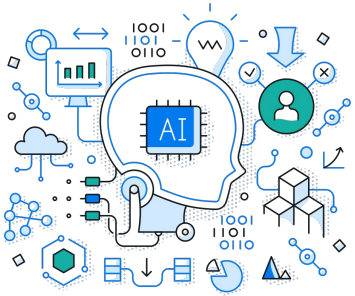
Enhancement of **monitoring** capabilities, improvement of process **understanding** and **integration** of new knowledge into efficient support systems, towards the development of a dedicated **Digital Twin Ocean** element

Project objectives

- to exploit the European Earth Observation (EO) capacity (primarily **Sentinel** and **Earth Explorer missions**)
- to develop **advanced tools** to combine and analyse satellite and in situ data, based on Artificial Intelligence/Machine Learning (AI/ML)
- to generate and validate **consistent high-resolution 4D reconstruction(s)** of the **Mediterranean Sea** physical and biogeochemical state
- to advance our understanding of the complex interactions between physical/biological/biogeochemical, **multi-scale processes** occurring in the Mediterranean Sea
- to demonstrate the **potential** of the project outcomes as **advanced monitoring solutions** for the management, restoration and preservation of the Mediterranean Sea Health







4DMED-sea

Proposed approach (1/3)

- the **development and generation** of **novel gap-free level 4 (L4)** **surface products** covering the Mediterranean Sea (2DMED): increased resolution surface **dynamic topography**, using AI 4Dvarnet algorithm (Fablet, 2021), and **sea surface salinity** (SSS) estimates, starting from the multivariate algorithm by Sammartino et al. (2022)

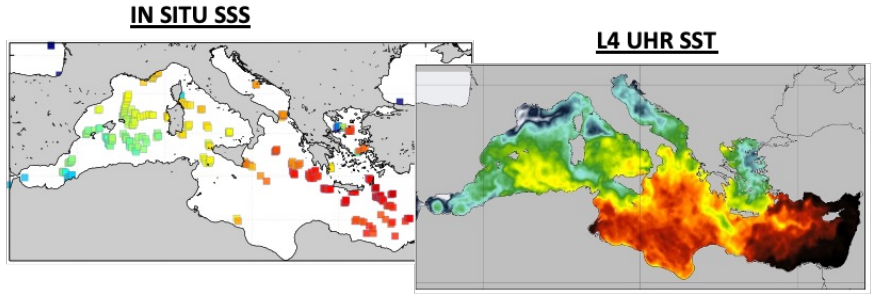
- the **development and generation** of **novel** **4D reconstructions** of both **physical** and **physical-biological ocean state** covering the Mediterranean (4DMED): different algorithms will be developed and tested, including AI/ML, deep learning approaches (e.g., Sammartino et al., 2020; Buongiorno Nardelli, 2020, Tréboutte, 2021). Bio-phys. reconstruction will also include estimations of the marine primary production with an upgraded version of the Morel (1991) model.

4DMED-sea

4DMED products: Sea Surface Salinity L4

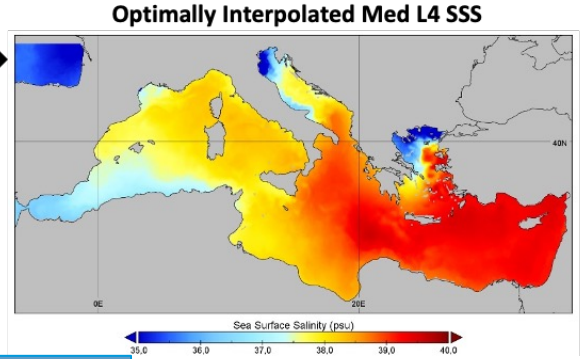
- Development of an **high resolution 2D Sea Surface Salinity (SSS) product** over the Mediterranean Sea, to be used as input to the 4DMED experimental processing chains;

- Validation of the new model for the production of the 2DMED SSS maps.



$$C(\Delta r, \Delta t, \Delta SST) = e^{-\left(\frac{\Delta r}{L}\right)^2} e^{-\left(\frac{\Delta t}{\tau}\right)^2} e^{-\left(\frac{\Delta SST_{filtered}}{T}\right)^2}$$

→Daily SSS L4 fields at 1/24° resolution based on the multivariate optimal algorithm developed by *Buongiorno Nardelli* (2012, 2016) and tested by *Sammartino et al.* (2022), which combines in situ, SMOS, SMAP, SST data.

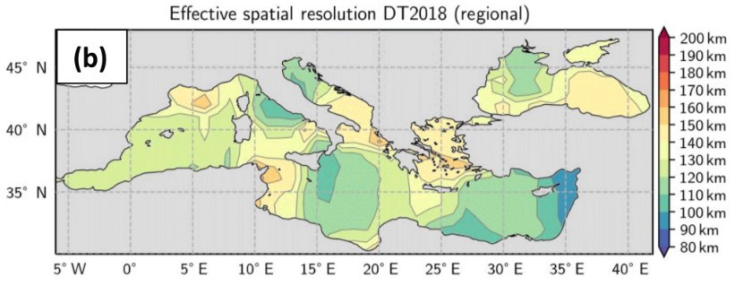


→Optimization of the interpolation model for the production of the 2DMED SSS maps:
- higher resolution (1/24° vs 1/16°)
- specific new mask for major rivers' mouth areas and North Adriatic Sea to combine monthly climatology and weekly global SSS used for the interpolation background field

4DMED products: Sea Surface Level L4

Sea surface level/absolute dynamic topography fields are needed to estimate geostrophic surface currents and to reconstruct the 3D temperature and salinity fields →the **spatial resolution of the sea level grids determines the horizontal scales of the 3D product**

- The operational mapping algorithm used in the operational Copernicus Marine Service SL production system (called DUACS), is an **objective analysis method, ingesting 1Hz** (7km) along track altimetric data to estimate daily regular grids with a 1/8° for the Med
- Transition to **MIOST** (**Multi-scale Inversion for Ocean Surface Topography**) solution developed since 2020 as part as several CNES R&D projects
- **AI method** today best candidate to propagate the small scale information far from the altimetry (swath) tracks



*Ballarotta et al..: On the resolutions of ocean altimetry maps, Ocean Sci., 15, 1091–1109, https://doi.org/10.5194/os-15-1091-2019, **2019**.*

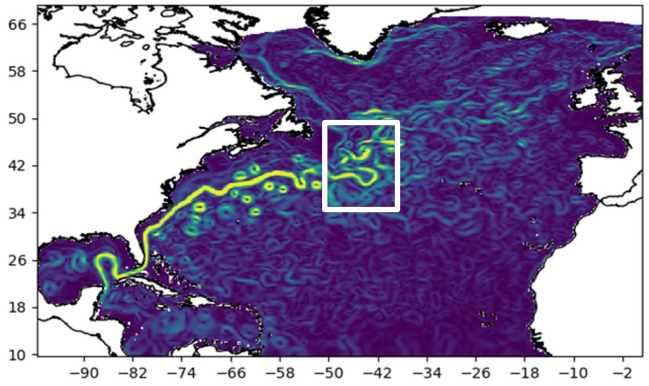
Objective of 4DMED: to develop a demonstration 2D Sea Level product over a 6-year period [2016-2021] with a refined posting (1/24°) an improved effective resolution, and assess its performance

Impact on the 4DMED project: Better consistency between 2D and discrete in situ vertical profiles to better resolve small mesocale ocean structures in the 3D products

4DMED-sea

Development of end-to-end learning frameworks for the 4dVarNet SL mapping

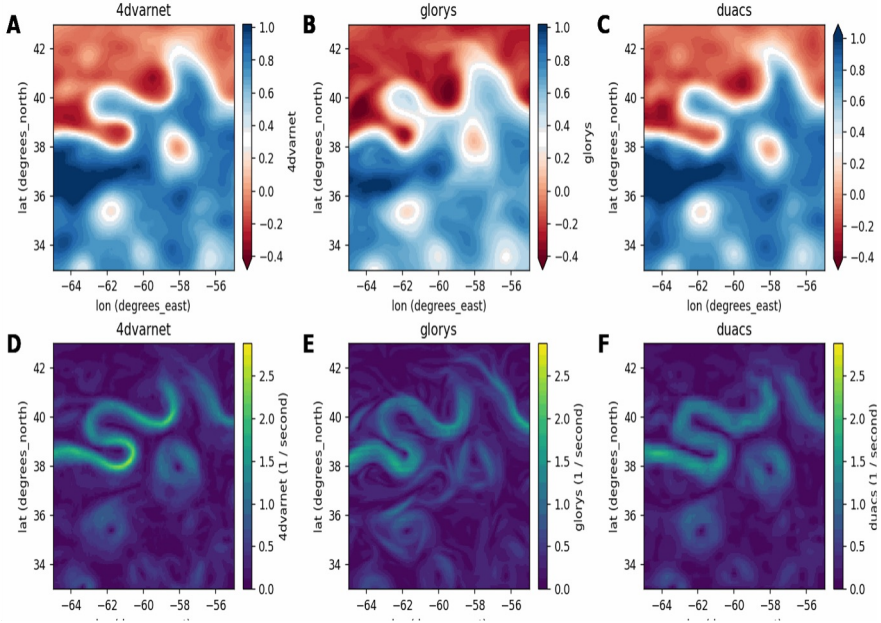
We propose here to apply and asses **the 4DVarNet framework developed by IMT Atlantique**, a deep learning scheme backed on a variational a trainable variational data assimilation formulation.



Fablet et al. Learning Variational Data Assimilation Models and Solvers. JAMES, 2021

Beauchamp, M., Febvre, Q., Georgenthum, H., and Fablet, R.: 4DVarNet-SSH: end-to-end learning of variational interpolation schemes for nadir and wide-swath satellite altimetry, Geosci. Model Dev., 16, 2119–2147, https://doi.org/10.5194/gmd-16-2119-2023, 2023.

4DVarNet, Glorys & DUACS SSH (and gradient) reconstructions over the Gulf Stream domain for 6 along-track real nadir datasets

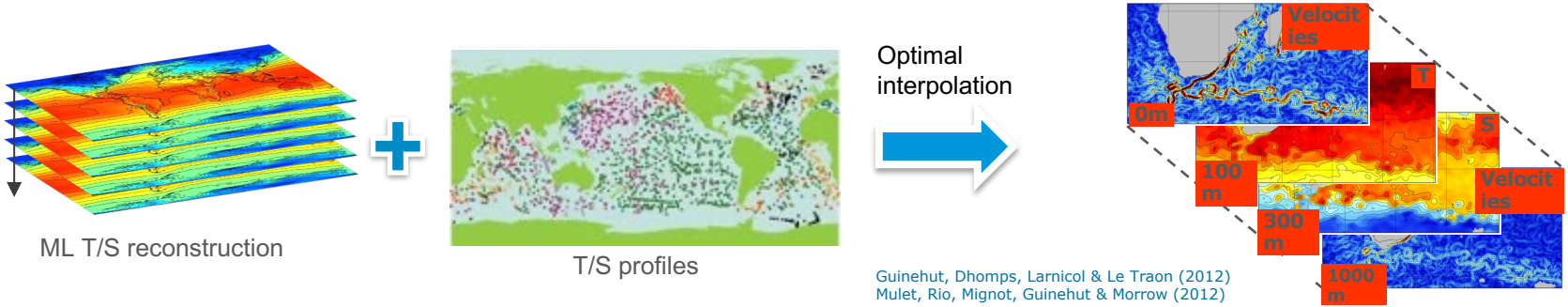


4DMED products: Experimental 4D physical variables

Novel 4D reconstructions of physical ocean state covering the Mediterranean (4DMED) through the synergic combination of HR L4 surface data and vertical profiles from in situ data.

key physical variables: T, S, MLD, Ug, Vg, through a three steps approach:

1. Machine learning approach to build T/S profiles
2. Correction of the large-scale residual biases by merging the T/S profiles reconstructed with in-situ T/S observations
3. MLD computation and geostrophic velocities computation by using the thermal wind equation



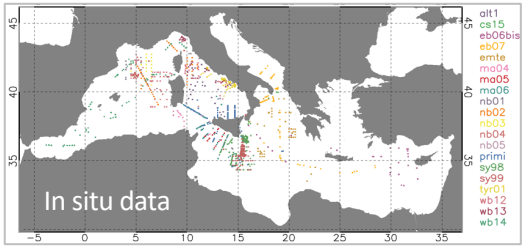
1. Machine learning process with a Multi-Layer Perceptron (MLP) model or more complex model (e.g. Tréboutte, 2021)

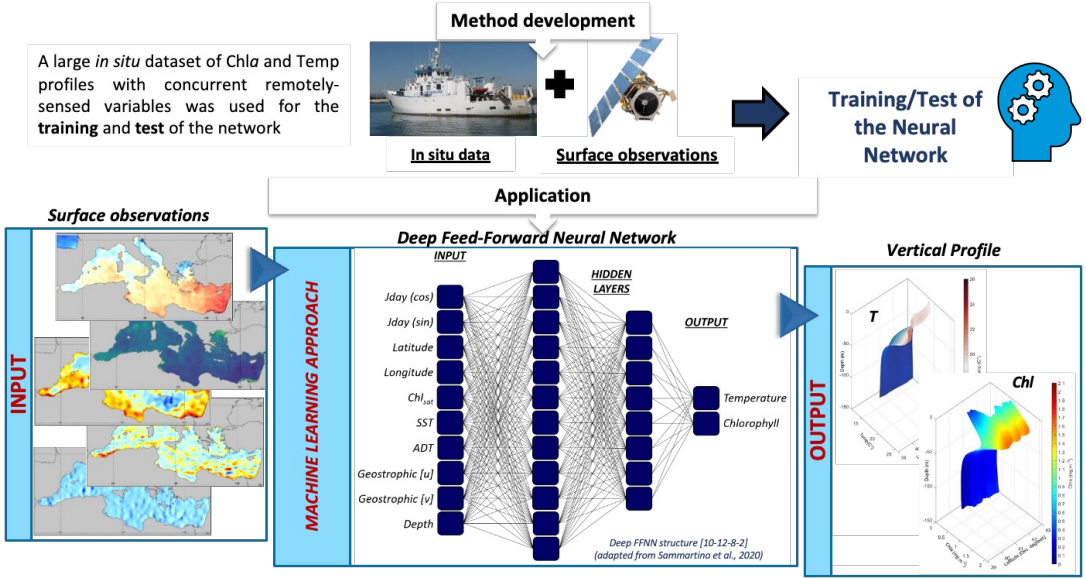
- *Target*: 4D fields from the Mercator-Ocean 1/12° global oceanic model with assimilation (used as a super-interpolator of observations)
- *Input*: ADT, SST, SSS + additional variables that will be tested to add context to local learning (Typically winds and/or 500dbar atmospheric pressure, Chl-a).
- Inferences will be done by using HR SSS & ADT 4DMED 2D products + other satellite observations and atmospheric data

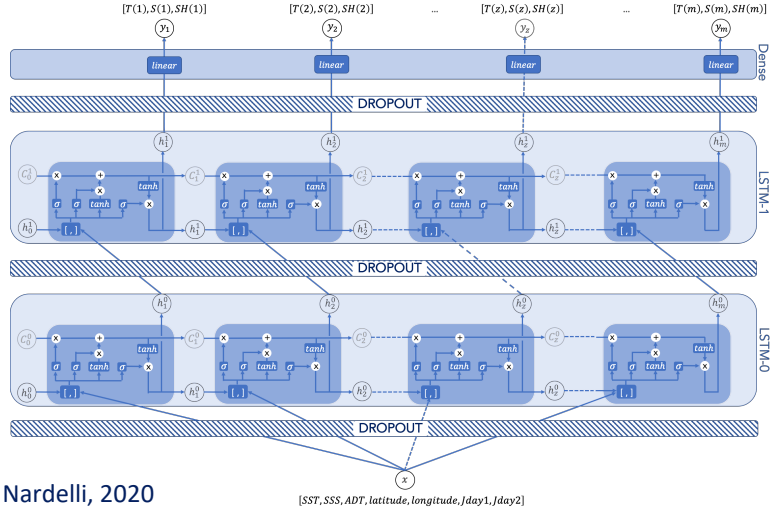
4DMED products: Experimental 4D combined physical-biological variables

Novel 4D reconstructions of physical-biological ocean state covering the Mediterranean (4DMED) through the synergic combination of HR L4 surface data and vertical profiles from in situ data

Develop/optimize an experimental **4DMED algorithm (based on AI)** providing a **joint 4D reconstruction** of key **physical** and **biological** variables (T, S, U_g, V_g, Chl-a, PP)







Sammartino et al., 2020; Buongiorno Nardelli, 2020

Proposed approach (2/3)

- the **development and application** of **advanced Lagrangian analysis and validation tools** including:

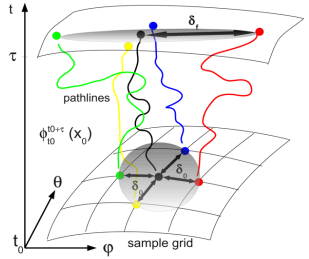
  -**Lagrangian models** incorporating inertial effects to compute trajectories of particles and tracers with different size, density, and behaviour (neural network approach, Hernandez-Carrasco and Orfila, 2018; kinematic approach, Lacorata et al., 2008; Falcini et al., 2015);

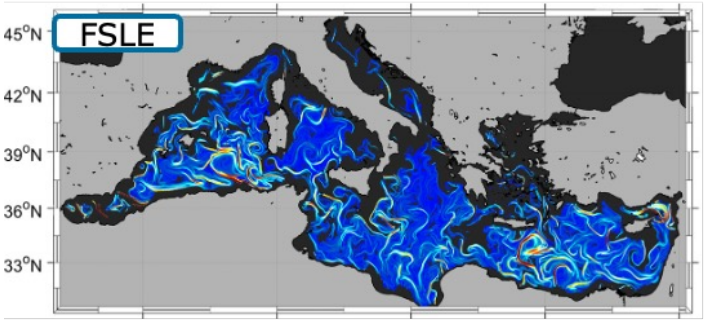
  -a suite of **Lagrangian metrics**

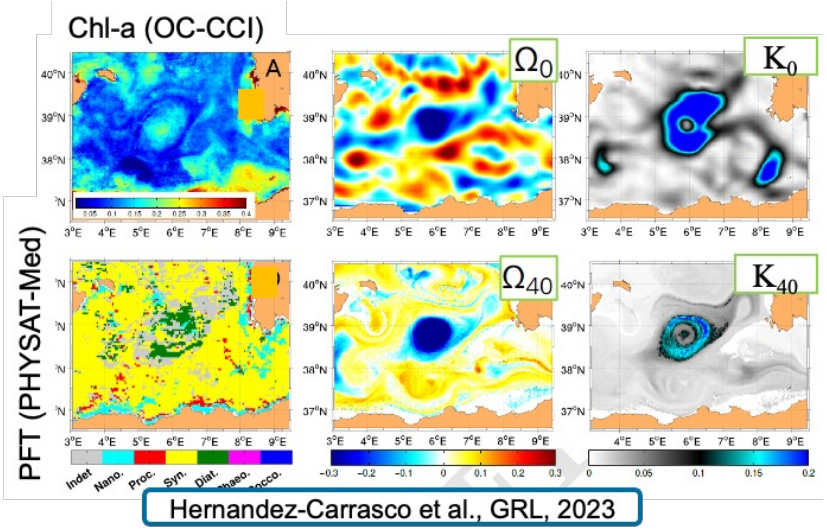
- an **intensive validation of experimental 2D/4DMED products** on the **western Mediterranean Sea** using physical and biological in situ observations collected from different experiments

Lagrangian analysis tools:

- Lagrangian coherent structures: Finite-size (Finite-time) Lyapunov Exponents.
- Lagrangian kinematic variables: Finite-time Lagrangian vorticity, Finite-Time Lagrangian EKE







Finite-time Lagrangian vorticity

$$\Omega_T(\mathbf{r}_0, t_0) = \frac{1}{T}\int_{t_0}^{t_0+T} \omega(\mathbf{R}_t(\mathbf{r}, t_0), t)\, dt$$

Finite-time Lagrangian EKE

$$K_T(\mathbf{r}_0, t_0) = \frac{1}{T}\int_{t_0}^{t_0+T} \kappa(\mathbf{R}_t(\mathbf{r}, t_0), t) dt$$

(Boffeta et al., 2001, d'Ovideo et al., 2004, Hernandez-Carrasco et al., 2011)

4DMED tools: validation

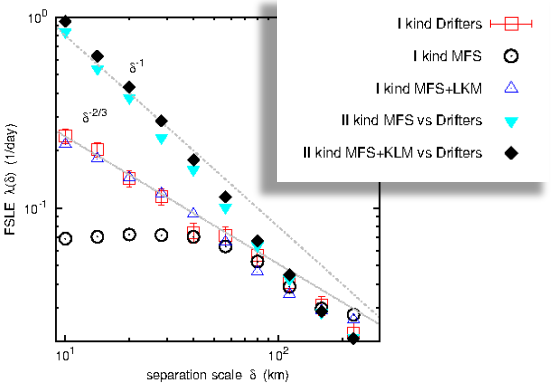
Lagrangian analysis tools:

Finite-Scale Lyapunov Exponent (FSLE) is an optimal indicator of relative dispersion properties providing a scale-dependent measure of the separation rate between two trajectories

I-kind FSLE: trajectories with the same dynamics (I-kind Predictability)

II-kind FSLE: trajectories with different dynamics (II-kind Predictability)

*How fast 4DMED trajectories separate from «real» trajectories and how the error growth rate changes with the scale of motion. If 4DMED and «real» trajectories start from the **same initial conditions** then, in the **early stage**, perturbations grow only for the effect of the **errors**.*



Lacorata et al., 2008; Falcini et al., 2015

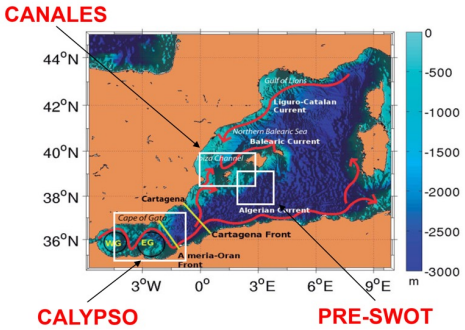
Intensive validation of experimental 2D/4DMED products:

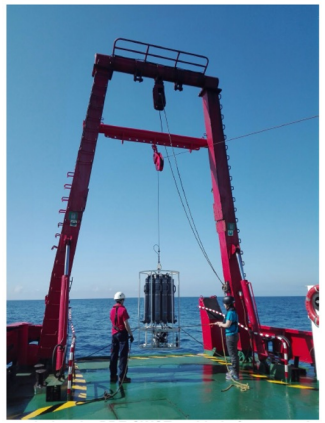
based on in situ multiplatform observations

- Ship-based CTD (Conductivity Temperature Depth) and ADCP (Acoustic Doppler Current Profiler)
- Gliders
- Drifters

Collected in 3 experiments:

- PRE-SWOT (Barceló-Llull et al., 2021)
- CANALES (Barceló-Llull et al., 2019)
- CALYPSO (Mahadevan et al., 2020)





Proposed approach (3/3)

- **three scientific case studies** aimed to:

1) improve our understanding of the **impact of mesoscale-to-submesoscale fronts on phytoplankton** organisms

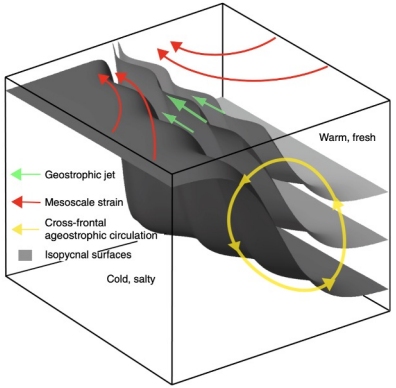
2) describe **Mediterranean seascape** and related variability in terms of **hydrodynamic provinces and biogeochemical/ecological regions**

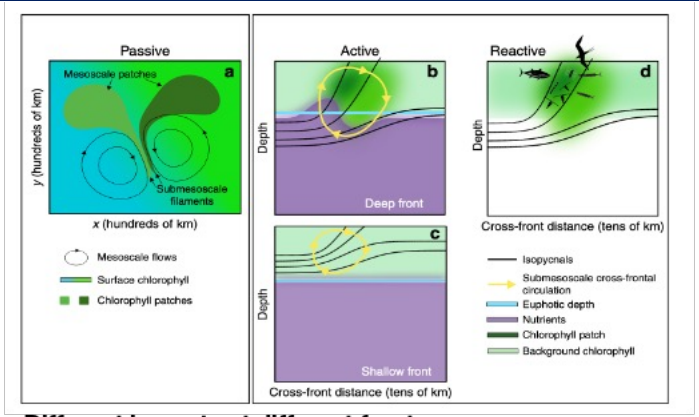
3) investigate **role of Lagrangian transport on the recruitment** of selected Mediterranean fish species

- **one test case** dedicated to:

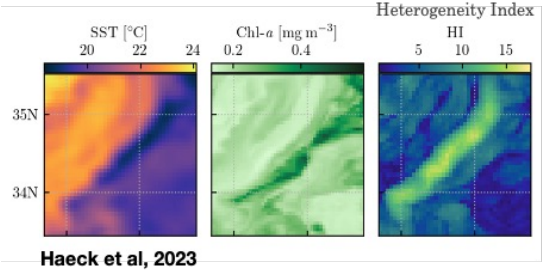
assess how 4DMED products and scientific results would fit into a **Digital Twin of the Ocean**, specifically targeting marine spatial planning/MPAs and fisheries management.

Scientific study case 1: Impact of fronts on phytoplankton distribution and diverstity



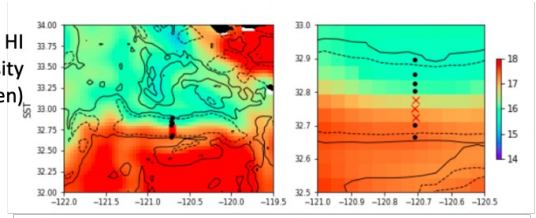


Different impacts at different fronts

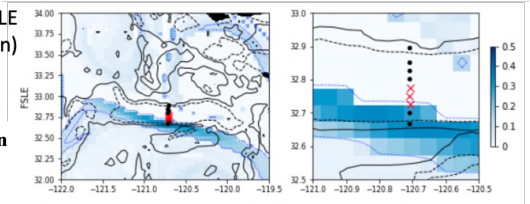


Haeck et al, 2023

From SST / HI
+ salinity = density
(Eulerien)



From SSH / FSLE
(Lagrangian)

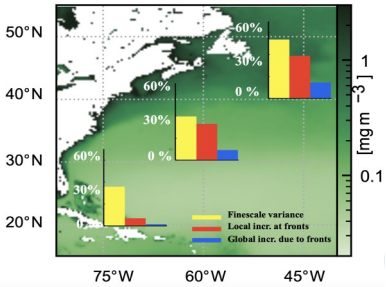


Objectives

1) Improve detection of fronts in the Mediterranean Sea
2) Seasonal variations of frontal activity in bioregions of the Mediterranean Sea
3) Quantify impact of these fronts on phytoplankton distribution and diversity

- Progressively update the front detection as new products become available along the project
- Compare Eulerien and Lagrangian Front detection
- Analyse Sub-surface fronts and Chl

Impact of fine-scales on phytoplankton



https://doi.org/10.5194/egusphere-2022-1489
Preprint. Discussion started: 6 January 2023

EGUsphere Preprint repository

marina.levy@locean.ipsl.fr

Satellite data reveal earlier and stronger phytoplankton blooms over fronts in the Gulf Stream region

Clément Haëck[1], Marina Lévy[1], Inès Mangolte[1], and Laurent Bopp[2]
[1]LOCEAN-IPSL, Sorbonne Université, CNRS, IRD, MNHN, Paris, France
[2]LMD-IPSL, École Normale Supérieure / Université PSL, CNRS, École Polytechnique, Paris, France

4DMED-sea

Partitioning the Mediterranean Sea in **ecoregions based on phytoplankton phenology and production**

extending classical approaches based on the analysis of the sole chlorophyll-a by including information on the composition of phytoplankton and organic carbon dynamics

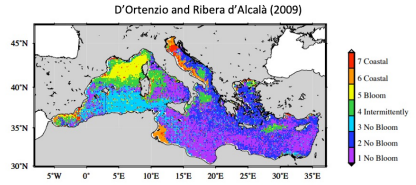
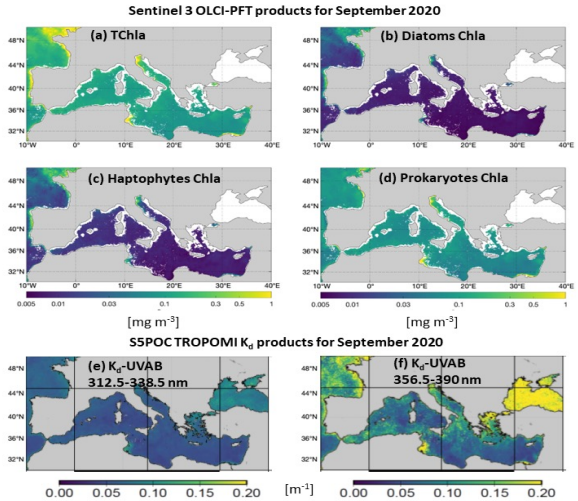
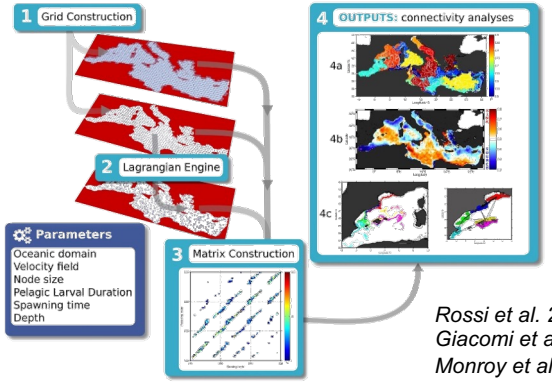


Fig. 4. Spatial distribution of the clusters obtained from the k-means analysis.

→focus on the 4DMed products, Sentinel 3 and 5P data



Partitioning the Mediterranean Sea in **ecoregions based on Lagrangian connectivity**

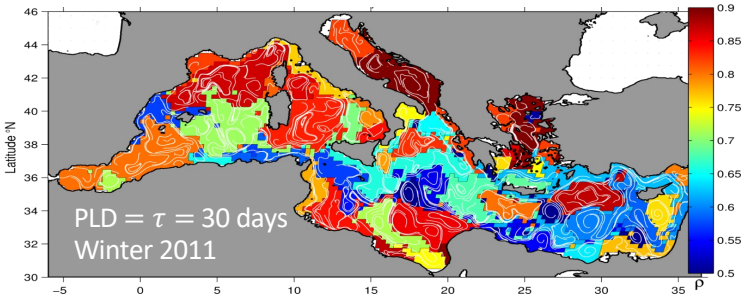


Rossi et al. 2014; Ser-Giacomi et al. 2015; Monroy et al. 2017

Lagrangian Flow Network
(Lagrangian model + network theory tools)

Community detection with ***Infomap***: finds the sets of nodes strongly connected among them and weakly connected with the rest

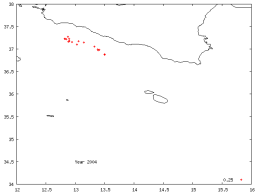
→ Hydrodynamical provinces in which larvae are more likely to disperse within each other than among them for a given time-scale



Scientific study case 3: role of Lagrangian transport on selected fish species recruitment

Anchovies in the Sicily Channel

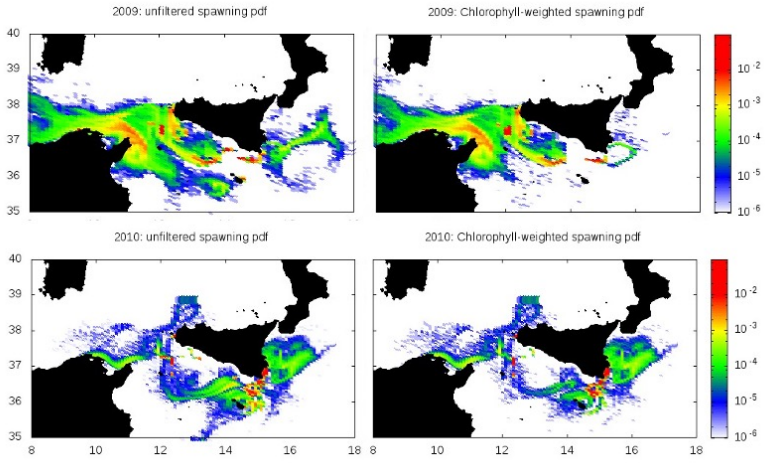
Ecosystemic connectivity from Lagrangian backtracking: starting from observed position of eggs or larvae



Chl (r) encountered by the larvae in their backward travel:

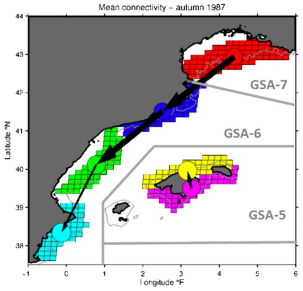
$$\bar{\rho}_i = \frac{1}{T}\int_{T}^{0} \mathrm{d}t\rho(\mathbf{x}_i(t))$$

Low survival below a fixed threshold:
pdf of zero-age position conditioned to $\bar{\rho} > \frac{1}{2}K$
(K = saturation value for anchovy larvae feeding)

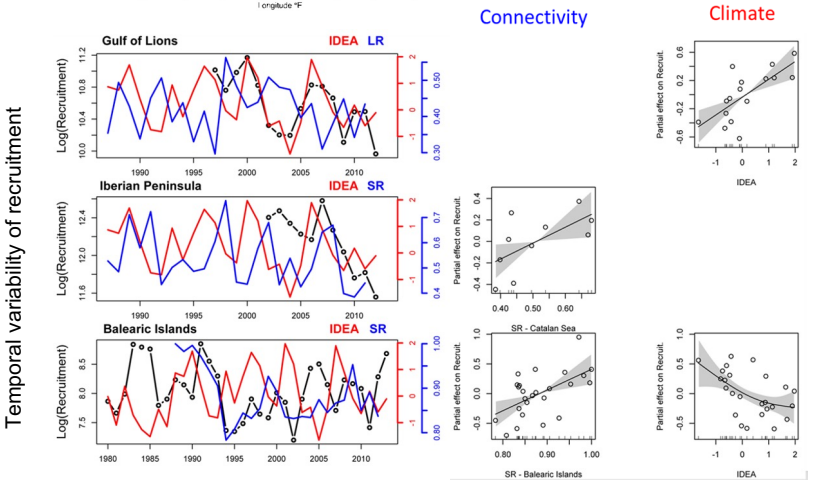


Hake larvae in Northwestern MED GSA

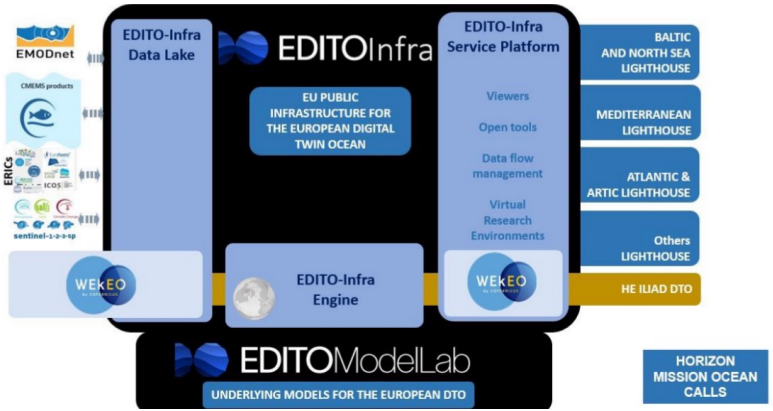
Investigate spatio-temporal variability of larval dispersal: compute various "connectivity metrics", exploit environmental information to capture "hydro-climate"



Inter-annual variability of exchange (arrows) and retention (circles)



Impact assessment use case: towards a DTO targeting MSP/MPAs and fisheries management



In order to transform 4DMED results into actionable information and to test the feasibility of a future integration in enhanced operational and decision support systems, the following requirements have been preliminarily identified:

- Identitification of the new assets produced by 4DMED
- Data format
- Associated metadata
- Description of the dissemination interface

Data standard shall allow for the creation of ARCO data and the associated metadata shall fullfill the minimum requirement for the inclusion in an advanced functionalities online catalogue

Steps:

1. Indentification of the general characteristics of the 4DMED generated assets
2. Agreement on the standard format associated to each assets
3. Agreement on the minimum set of metadata associated
4. Integration test

Recommendations to ESA

1. Recent Achievements

- 4DMED-Sea still in initial phase

2. Identified gaps

- need for properly designed and openly shared data for AI model developments and intercomparison
- ever-growing number of possible models to be tested for different objectives require more time than currently available within 2-year ESA projects
- 4DMED dynamics could not tackle vertical component (too much effort required)

3. Gap-filling Opportunities

a. Short-term

- open data challenges (co-designed)
- cross-fertilization between projects

b. Long-term

- extend/expand diagnostic models to full 3D dynamics

4. Additional remarks/notes/hints/recommendations

- Reduce number of objectives per project in future tenders (extremely challenging)
- Scientific studies would require longer time also to be able to attract dedicated personnel (PostDoc)

Thank you!