SERVICES BASED ON ECOSYSTEM DATA ASSIMILATION: ESSENTIAL SCIENCE AND SOLUTIONS (SEAMLESS) WAYS OF EXPLOITATION BY CMEMS

Stefano Ciavatta on the behalf of the SEAMLESS team

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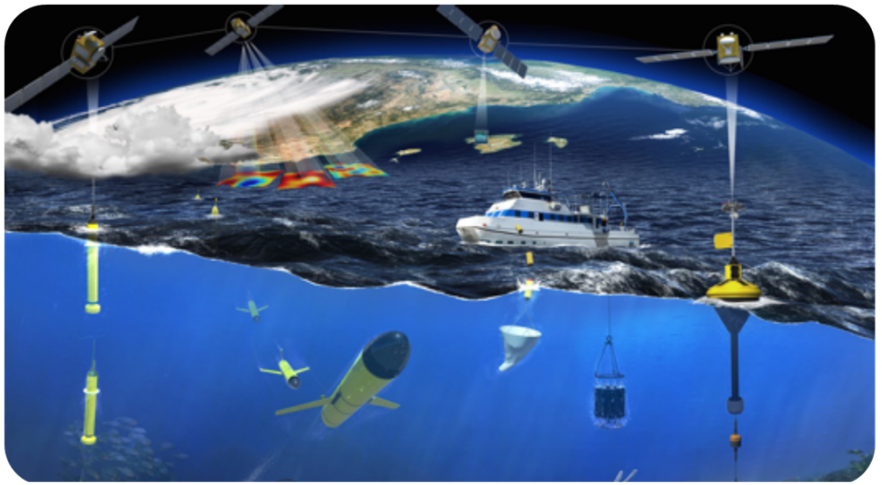
STAC Meting Nov 2022

Vision and mission

Copernicus Marine Service

Vision
to support sustainable food-security
from the ocean in a changing climate



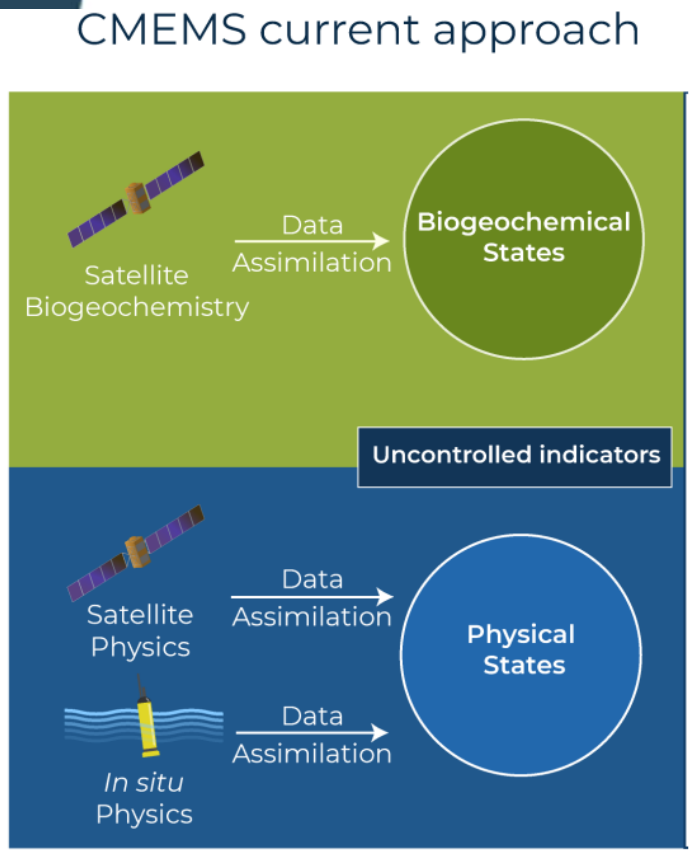
Mission
to improve the operational simulation
of indicators related to climate impact,
marine food-webs and stakeholders' needs

Objective of this talk
To give MOi and STAC an overview and
the flavor of what CMEMS could up-take

A predicted ocean

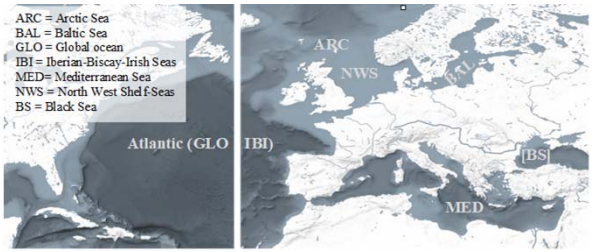
2021 2030 United Nations Decade of Ocean Science for Sustainable Development

Science overview



Hypothesis: New integrated observing networks and advanced ensemble data assimilation methods can improve the simulation of marine ecosystem indicators (i.e. increase their observability, controllability and identifiability)

The four research streams



BGC models: PISCES, ERSEM, BFM, ECOSMO, ERGOM, [BAHMBI]

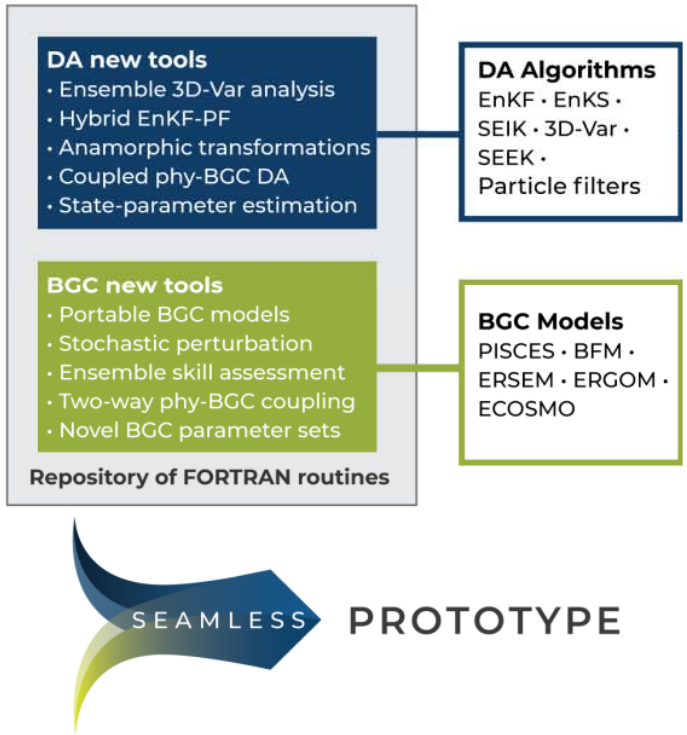
1. New ensemble generation and data assimilation methods (WP3, P Brasseur, UGA)
   to maximize the flow of information from the new observing networks towards the controllable ecosystem indicators

2. Coupled assimilation of physical and biogeochemical data (WP4, L Bertino, NERSC)
   to improve the consistency of the biogeochemical and physical simulations

3. Coupled assimilation of remote sensing & in situ biogeochemical data (WP5, Cossarini, OGS)
   to link the surface and subsurface ecosystem dynamics

4. Coupled assimilation for joint state-parameter estimation (WP6, J Skakala)
   to improve the models and their simulation of biogeochemical indicators.

WP2 The SEAMLESS prototype: EAT (Ensemble and Assimilation Tool)



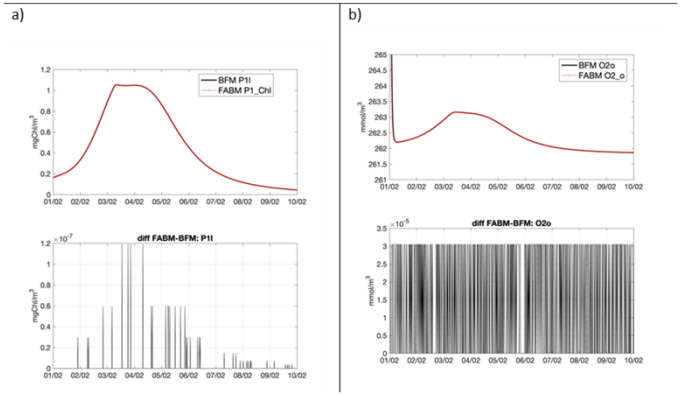
https://github.com/BoldingBruggeman/eat

Deliverable D2.1 “Prototype core system”

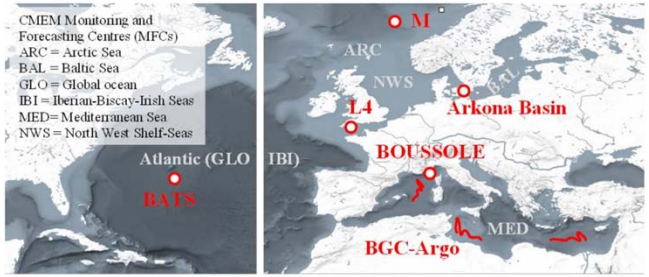
WP2 Prototype Highlights

- Developed **EAT** (Ensemble and Assimilation Tool) for 1D prototype
  - Coupling GOTM, BGC models (leveraging **FABM**) and PDAF
- **Enhanced PDAF** to include both ensemble filters/smoothers and 3D-Var methods including ensemble and hybrid 3D-Var
- Will be made available as **open source** with full documentation
- Plan to utilize EAT in **training** sessions
- Allows comparison studies using data assimilation und sensitivity analysis
  - **Multi-model ensembles**
  - e.g. compare **sensitivities** of different BGC models to process parameters using identical physical environments
  - e.g. apply different **data assimilation** methods under identical modelling conditions

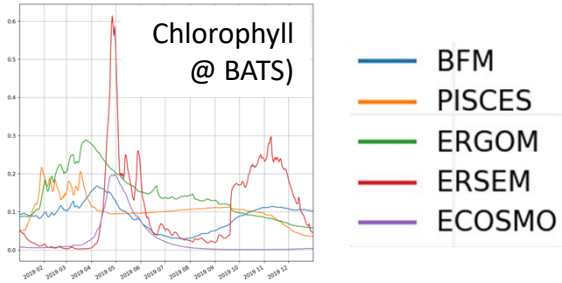
Implementation and test of BFM in FABM



Testing the prototype in monitoring sites

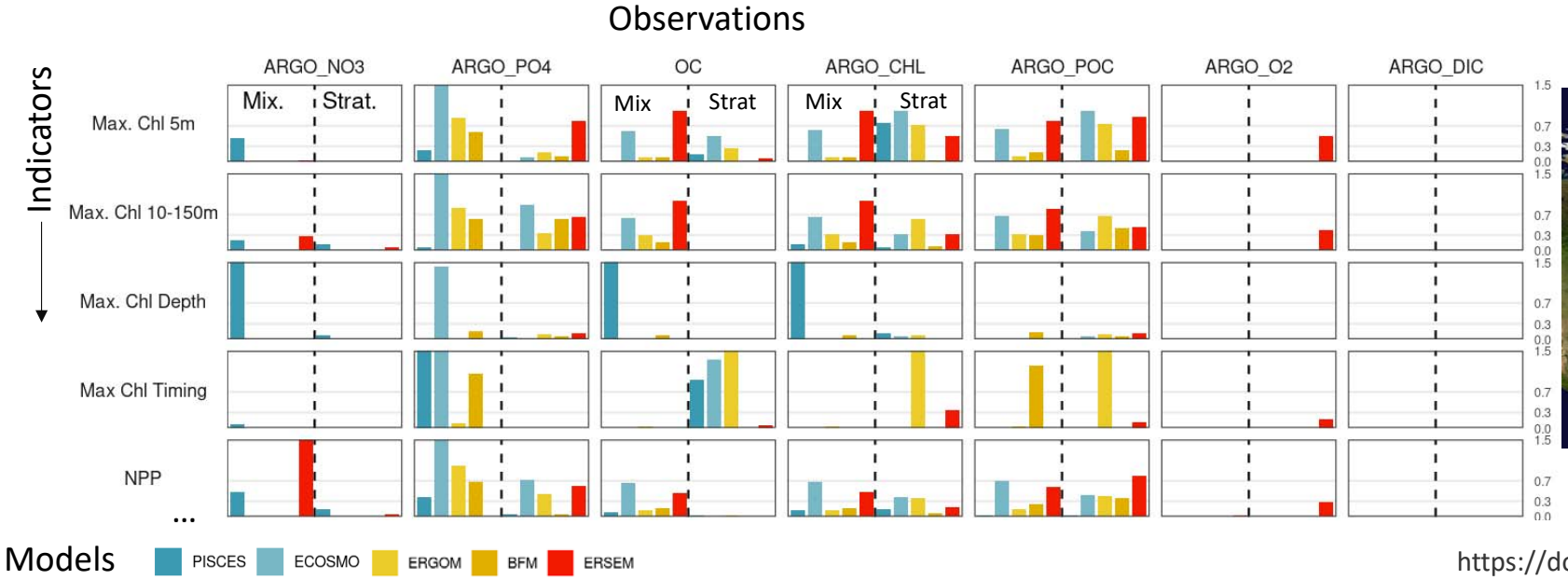


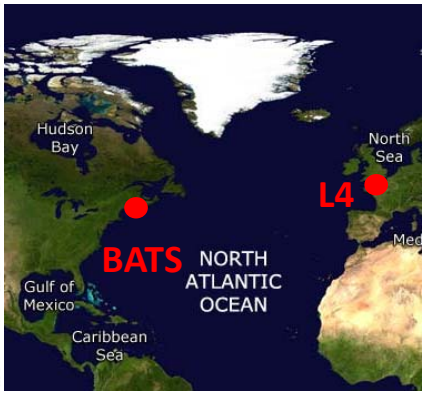
Multi-model ensembles



Lazzari, et al., 2021, Deliverable 2.2, Doi: 10.5281/zenodo.6401395

WP3 - Sensitivity (controllability) of ecosystem indicators to the obs & parameters





Ciavatta et al., 2022,
SEAMLESS, Project report,
https://doi.org/10.5281/zenodo.6580236

PISCES				
Rank	Notation	Description	Score	Group
1	dom_rem/xremik	DOM remineralization rate	100%	[10]
2	dom_rem/xkdoc	DOC half-saturation constant in limiting bacterial DOM degradation activity (Aumont et al, Eq 34)	99%	[12]
3	Optics/parlux	PAR : SWR ratio	93%	[6]
4	zoo/xprefn	Microzooplankton preference for nanophyto	91%	[17]
5	Dia/mumax0	Diatoms Max Growth	90%	[1]
6	Phy/logbp	Nanophyto temperature sensitivity for growth	88%	[5]
7	zoo/grazrat	MicroZoo maximum grazing rate	85%	[13]
8	phy/mumax0	Nanophyto Max Growth	83%	[1]
9	dia/logbp	Diatoms Temperature sensitivity for growth	81%	[5]
10	phy/padlopers	Nanophyto P-I slope	67%	[1]

ERSEM				
Rank	Notation	Description	Score	Group
Group				
1	light/PEIR_eow,	photosynthetically active fraction of shortwave radiation,	100%	[6]
2	B1/pu	efficiency at high oxygen levels (bacteria)	92%	[9]
3	B1/sR1	maximum turn-over rate of DOM	83%	[12]
4	light/a0w	absorption coefficient of clear water	74%	[21]
5	B1/rR2	fraction of semi-labile DOC available to bacteria	69%	[12]
6	P2/xqcn	threshold for nitrogen limitation (relative to Redfield ratio) in nanophytoplankton	61%	[20]
7	P1/xqn	maximum nitrogen to carbon ratio (relative to Redfield ratio) for diatoms	58%	[20]
8	P1/xqcn	threshold for nitrogen limitation (relative to Redfield ratio) in diatoms	57%	[20]
9	P2/xqn	maximum nitrogen to carbon ratio (relative to Redfield ratio) for nanophytoplankton	57%	[20]

WP3 - Ensemble generation and assimilation methods

Relevant problem for CMEMS

- **Robust information about product uncertainties is needed by users** to help in decision-making and management of marine ecosystems.
- In today's CMEMS catalogue, **most BGC products generated by MFCs do not contain uncertainty estimates.**
- In WP3, we demonstrate that **a transition towards ensemble assimilation methods with uncertainty estimation capabilities is feasible in all MFCs** for real time, delayed mode and forecast mode BGC products with a few days of lead time.

Explored methods

- EnKF / EnKS
- Hybrid Ensemble / NEMOVAR
- Hybrid EnKF / Particle filter
- Stochastic Ensemble filter/smoother
- SEIK filter

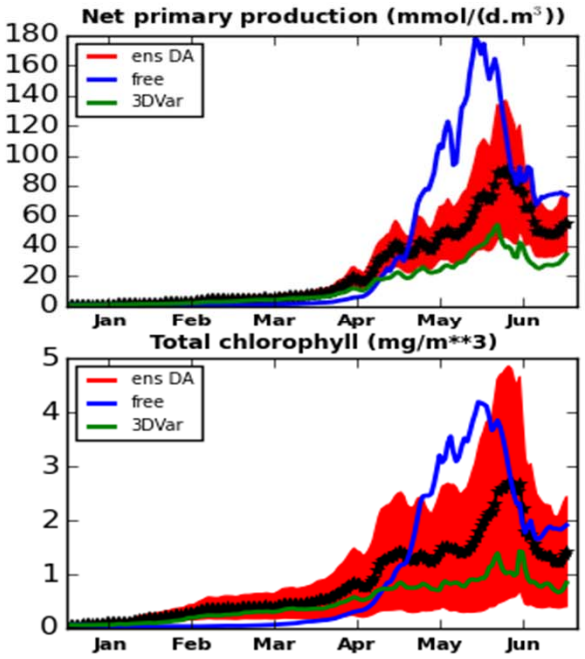
1 Global
2 Arctic
3 Baltic
4 NWS
5 IBI
6 Med Sea
7 Black Sea

SEAMLESS

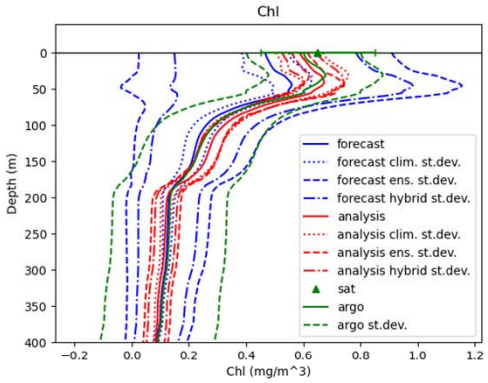
ODESSA

WP3 – Scientific highlights (II)

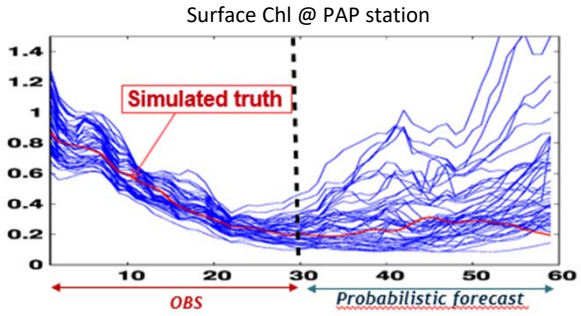
- ***Uncertainty reduction using ensemble DA methods***



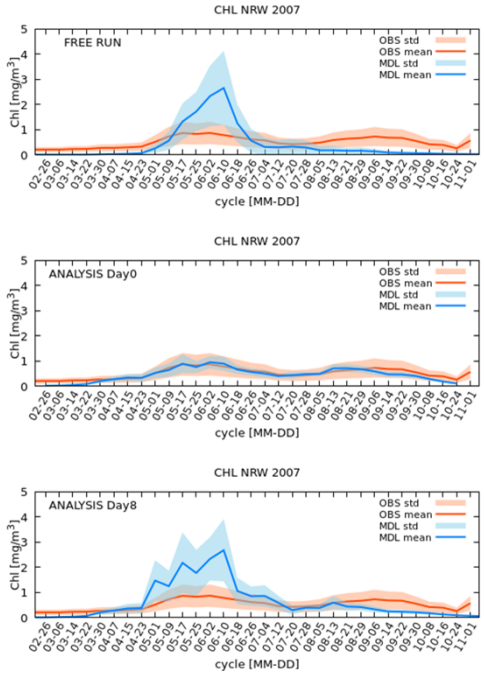
In hindcast mode (NWS)



On the vertical (MED)



In forecast mode (IBI/GLO)



In real-time mode (ARC)

Brasseur P. *et al.* (2022). D3.4 Observability of the target indicators in the 3D CMEMS MFC systems.

WP3 – Take-home messages for system design

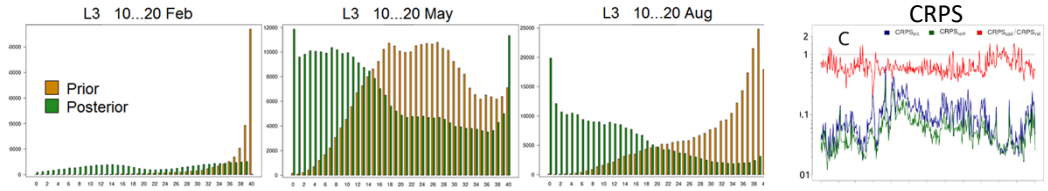
1) **Strategy for dealing with uncertainty sources:** priority on uncertain BGC model parameters, but biases generated by the physics remain an issue

2) **Transition to ensemble monitoring and forecasting system in MFCs:** can be envisaged in an incremental way, with a first step consisting in simulating ensembles

3) **Optimal complexity level of BGC models:** increasing model complexity does not necessarily increase robustness and reliability of estimates

4) **Choice of numerical settings and assimilation methods:** ensemble approaches imply to reconsider a number of modelling choices (e.g. resolution) made previously with respect to assimilation cost constraints, especially for coupled physical-BGC systems.

5) **Ensemble diagnostics and data sets :** split between verification and assimilation data sets + adopt standard metrics already developed in the NWP community



Brasseur *et al.* (2022) D3.1 doi: 10.5281/zenodo.6390306

Brasseur *et al.* (2022) D3.4

Indicator	ARC	BAL	NWES	MED	GLO/IBI
Phenology	High		High	Medium	High
PP	n/a		High	Medium	Medium
POC flux	n/a		High	Low	Medium
PFT	Medium		Medium	Medium	n/a
Trophic efficiency	Medium		High	Low	Low

Table 5.2. Assessment of observability/controllability levels of ecosystem indicators in the 5 CMEMS regions

WP4 Objectives

- Operational bio-modelling systems *do not draw the maximum benefit* from assimilation of physical data, some even suffer deterioration of the biogeochemistry.
- The overall objective of WP4 is to remove a blocking point for the mutual consistency of physical and BGC assimilation practices in CMEMS

Timeline:

Start Apr. 2022 -> End Dec. 2022 (fresh results, need consolidation)

2 Tasks

> Task 4.1 Weakly coupled assimilation (AWI, OGS, PML, UGA)
> Task 4.2 Strongly coupled DA (NERSC, AWI, PML, IGE)

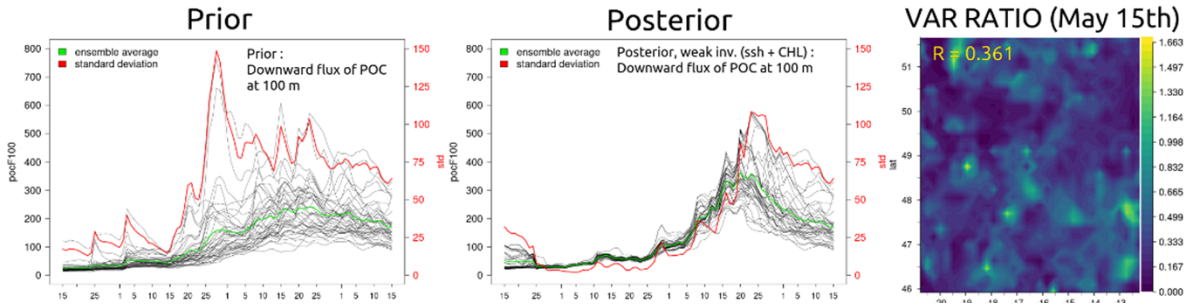
Summary table

Who	Where 1D	Where 3D	DA method in CMEMS	Weakly Coupled DA	Strongly Coupled DA
AWI	Arkona	BAL	LESTKF (fixed ensemble)	Ensemble	Ensemble
IGE	/	Atl. (GLO/IBI)	SEEK (fixed ensemble)	Ensemble (4D LETKF)	Ensemble
NERSC	Station M	/	EnKS	/	Ensemble (EnKF)
OGS	Boussole	MED	3DVAR	Ensemble (PHY)* 3D VAR (BGC)	/
PML	L4	NWS	3DVAR	Hybrid Ens.-3DVAR*	3DVAR (3D)

*: New method for the team
Experiments still ongoing

(WP4) Weakly coupled assimilation

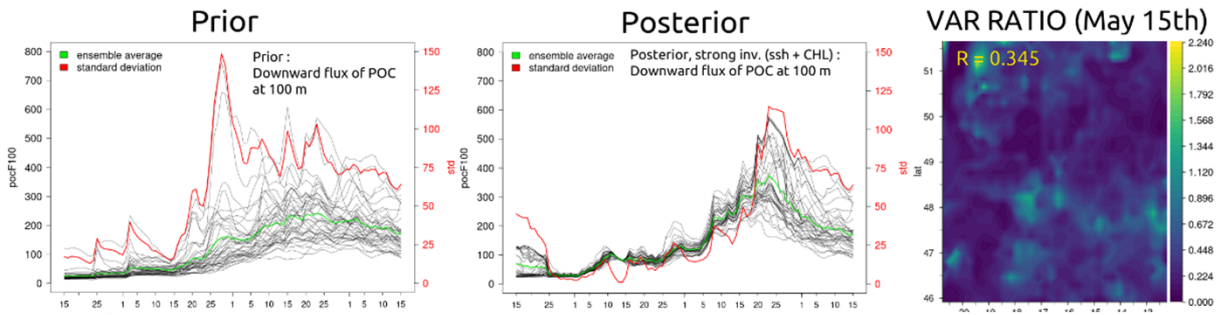
- MED (OGS): PHY assimilation increments -> nutrients (Background covariance in 3DVAR)
  - Data from BGC Argo
  - Positive influence from prescribed covariances, but not ensemble covariances
- IBI/GLO (UGA): Long window 4D ensemble smoother
  - 1st step for PHY (altimeters), 2nd step for BGC
  - Small effect, but no degradations
- NWS (PML): Hybrid Ens-Var 3DVAR
  - Dynamical ensemble leads to BGC deterioration
- BAL (AWI): To be completed



Indicator	ARC	BAL	NWS	IBI/GLO	MED
Phenology	-		Moderate degradation (glider data)	Moderate improvement (Chl from OC)	Moderate improvement (Chl from BGC-Argo)
PP	-		N/A	Changes	Improvement (Chl and NO3 from BGC-Argo)
POC flux	-		N/A	Changes	Changes
PFT	-		Changes	N/A	Changes
Trophic efficiency	-		Changes	Changes	Changes
pH	-		N/A	N/A	N/A
O	-		Changes	N/A	N/A

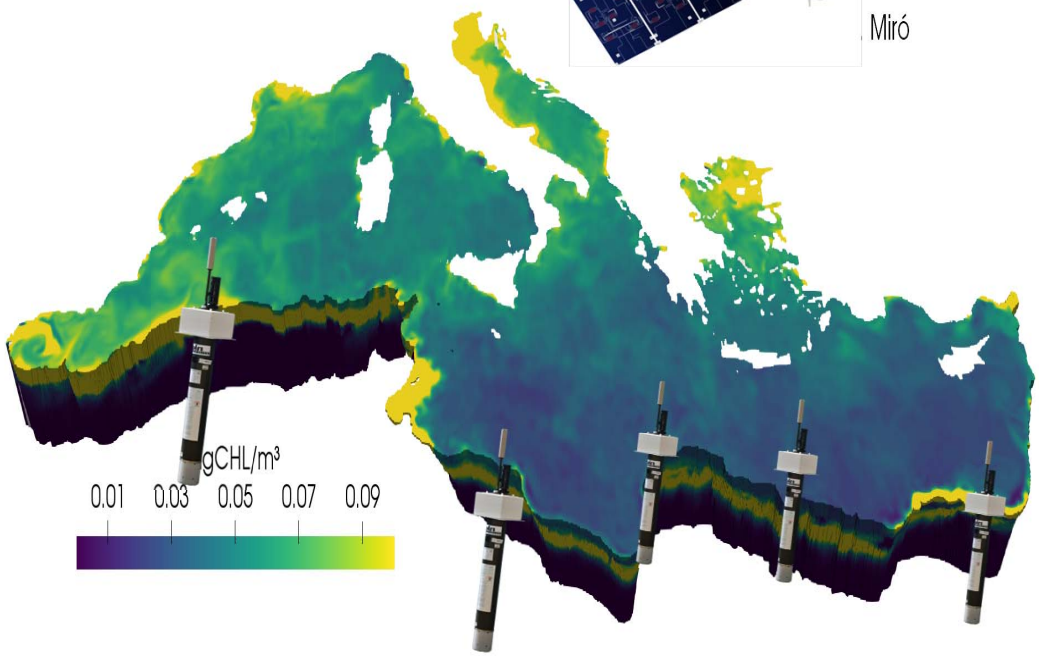
Strongly coupled assimilation

- IBI/GLO (UGA): Long window 4D ensemble smoother
  - One step for PHY (altimeters) and BGC (OC)
  - Small effect, but no degradations
- NWS (PML): Hybrid Ens-Var 3DVAR
  - Dynamical ensemble leads to BGC deterioration
- ARC (NERSC): To be completed
- BAL (AWI): To be completed



Indicator	Weakly coupled	Strongly coupled
Surface chlorophyll concentration	0,321	0,205
Particulate Organic Carbon flux	0,361	0,345
Trophic Efficiency	0,163	0,147
Net Primary Production	0,233	0,224

Operational bio-modelling systems commonly assimilates only Remote Sensing data (mostly chlorophyll). New observing systems (BGC-Argo floats, Gliders and buoys) capabilities are emerging



WP5 objectives:

- The overall objective of WP5 is to enhance DA capabilities (ensemble methods) to **better** link **the surface and subsurface ecosystem dynamics**
- **SEAMLESS will enable CMEMS MFCs to assimilate biogeochemical observations from the Copernicus space element and *in situ* platforms consistently, to link better the surface and subsurface ecosystem dynamics to water quality, carbon cycle and food web indicators**

Hypothesis:

Ensembles maximizing the flow of information across the discretized vertical dimension of the model domain can provide information to constrain BGC variables at the **ocean surface and interior consistently**

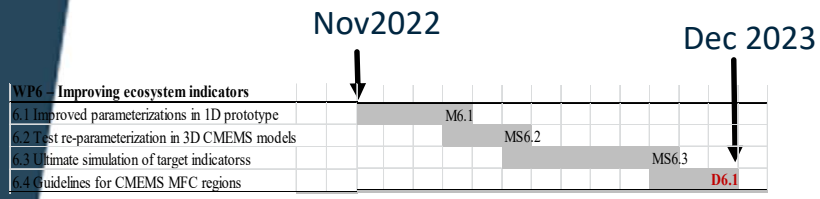
Partner	CMEMS MFC	Assimilated variables			Ensemble data assimilation methods in 1D and 3D systems
		Remote sensing data	Profiles in 1D experiments	Profiles in 3D experiments	
NERSC	ARC	Chlorophyll from CMEMS OC TAC	Chlorophyll from BGC-Argo	Chlorophyll from BGC-Argo and nutrient profiles from CMEMS INSITU TAC	ENKF
PML Plymouth Marine Laboratory	NWS	PFT chlorophyll from CMEMS OC TAC	Temp, chlorophyll, oxygen from L4 and semi-synthetic profiles	Temp., Sal, Chlorophyll, oxygen, from EN4 (Hadley data-set) + glider	Ensemble-3DVAR
OGS National Institute of Oceanography and Applied Geophysics	MED	Chlorophyll from CMEMS OC TAC	Chlorophyll and nitrate from BGC-Argo	Chlorophyll and nitrate from BGC-Argo floats	SEIK

- The 1D prototype system will be used as proof-of-concept for assessing multiplatform assimilation combining different types of observations and testing different options
- The 3D MFC models with the methods developed in WP3 will be used to test the assimilation of the multiplatform observations

Aspects to be investigated:

- impact of the assimilation of new sensors
- frequency of the ocean colour assimilation
- tuning of the observation errors for ocean colour and profiles of the same variable
- vertical spatial resolution of profile observations

WP6: the relevant problem addressed is to <u>improve the MFC biogeochemical models through better parametrization</u>



T6.1: identify better parameter values through joint parameter-state estimation in 1D

T6.2: test and validate these parameters in a corresponding 3D run

T6.3: choose the best configuration and produce the improved reanalyses for the target indicators

Table for T6.1: estimating improved parameter values

Partner	1D model	DA scheme	Parameters	assimilated data	station	period
OGS	GOTM-FABM-BFM	EnKF	Most sensitive obtained from WP3	Chl satellite + in-situ, NO3 in-situ	BGC-Argo in Mediterranean Sea	2019
NERSC	GOTM-ECOSMO	EnKF	Most sensitive obtained from WP3	Satellite Chl-a	BGC-Argo in Norwegian Sea (close to StM)	2019
PML	GOTM-ERSEM	Ensemble-3DVAR	3-6 most sensitive from WP3	SST and PFT chl satellite+L4 T, chl, o2 in situ	L4	1 year, Nov 2014-Oct 2015
AWI	GOTM-ERGOM	ESTKF	tbd.	tbd.	Arcona	1 year

Dissemination and communication

- Find out details and update on the project website: https://seamlessproject.org/
- Details of SEAMLESS prototype – an open-source, user-friendly assimilative modelling tool available through website
- Programme of hands-on training events coming soon.
- Organisation and participation in workshops to share and disseminate project developments across the community, including:
  - Co-organization of the BGC-DAWG meeting
  - CMEMS General Assembly

- Skakala et al, JGR (2021)
- Skakala et al, OM (2022)
- Ford et al, Frontiers, in review

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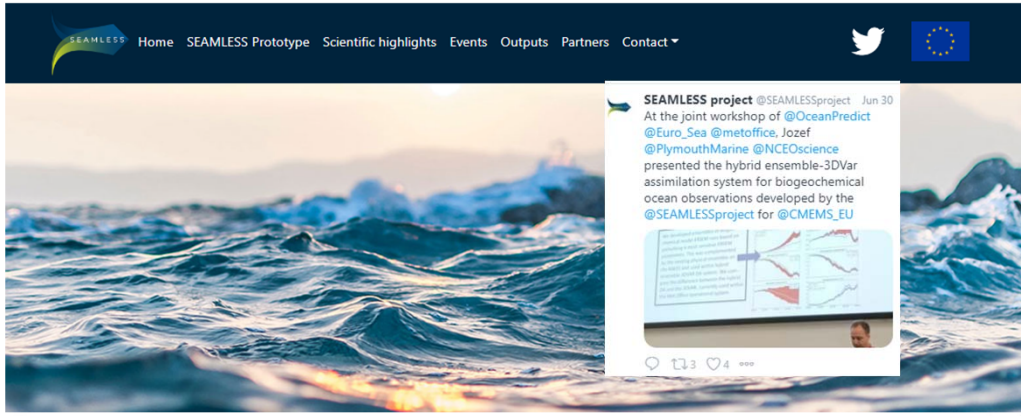

Services based on Ecosystem data AssiMiLation: Essential Science and Solutions (SEAMLESS)

SEAMLESS aims at improving the current European capability to simulate and predict the state of marine ecosystems. The project focuses on state indicators that are linked to the ocean "health" (e.g. to oxygenation, acidification, eutrophication), "services" (e.g. to ocean depths). Currently, these ean Copernicus Marine Services from monitored and simulated

SEAMLESS Prototype

SEAMLESS has developed an **open-source, user-friendly assimilative modelling tool: the "SEAMLESS prototype".**

The core system of the prototype is a software made up of a 1-dimensional physical model coupled to five biogeochemical models and enabled with data-assimilation capabilities. The five biogeochemical models are used operationally in the Copernicus Marine Service, namely: PISCES, ERSEM, BFM, ECOSMO and ERGOM.

We have named to prototype EAT (SEAMLESS Ensemble and Assimilation Tool) (EAT) and it is publicly available on GitHub via – https://github.com/BoldingBruggeman/eat. EAT will be continually developed over the next few years of the SEAMLESS project and the GitHub page will always have the authoritative version.

EAT builds on other software projects – notably General Ocean Turbulence Model (GOTM – https://gotm.net), Framework for Aquatic Biogeochemical Models (FABM - https://fabm.net) and the Parallel Data Assimilation Framework (PDAF – http://pdaf.awi.de) and integrates these different components into a software product capable of doing data-assimilation simulations for any GOTM configuration where observations are available.

EAT will not only be a development platform for testing new assimilation methods and new biogeochemical models – but – also a production ready assimilation system for realistic 1D setups.

Related links

EAT (SEAMLESS Ensemble and Assimilation Tool)

General Ocean Turbulence Model (GOTM)

Framework for Aquatic Biogeochemical Models (FABM)

Parallel Data Assimilation Framework (PDAF)

odel data to:

Investigate climate change impacts on ocean ecosystems

Acknowledgements

PML | Plymouth Marine Laboratory

UGA Université Grenoble Alpes

AWI

Bolding & Bruggeman

OGS

NERSC

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