From surface optics to subsurface ecosystem structure

how reflectance assimilation propagates beyond biogeochemistry

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Ocean Insights for the Future

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NEW COPERNICUS CAPABILITY FOR TROPHIC OCEAN NETWORKS

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The problem

ocean-colour retrievals inject algorithm error into the assimilated state

5–40%

OC chlorophyll retrieval error, open ocean

100–300%

in optically complex coastal waters

Ciavatta 2011, 2018; Pradhan 2020; Jones 2016

Error chain:



Solution: *assimilate the reflectance itself through a forward RT model — require a complex RT representation*

The approach

follow numerical weather prediction — assimilate the measurement, not its derivatives

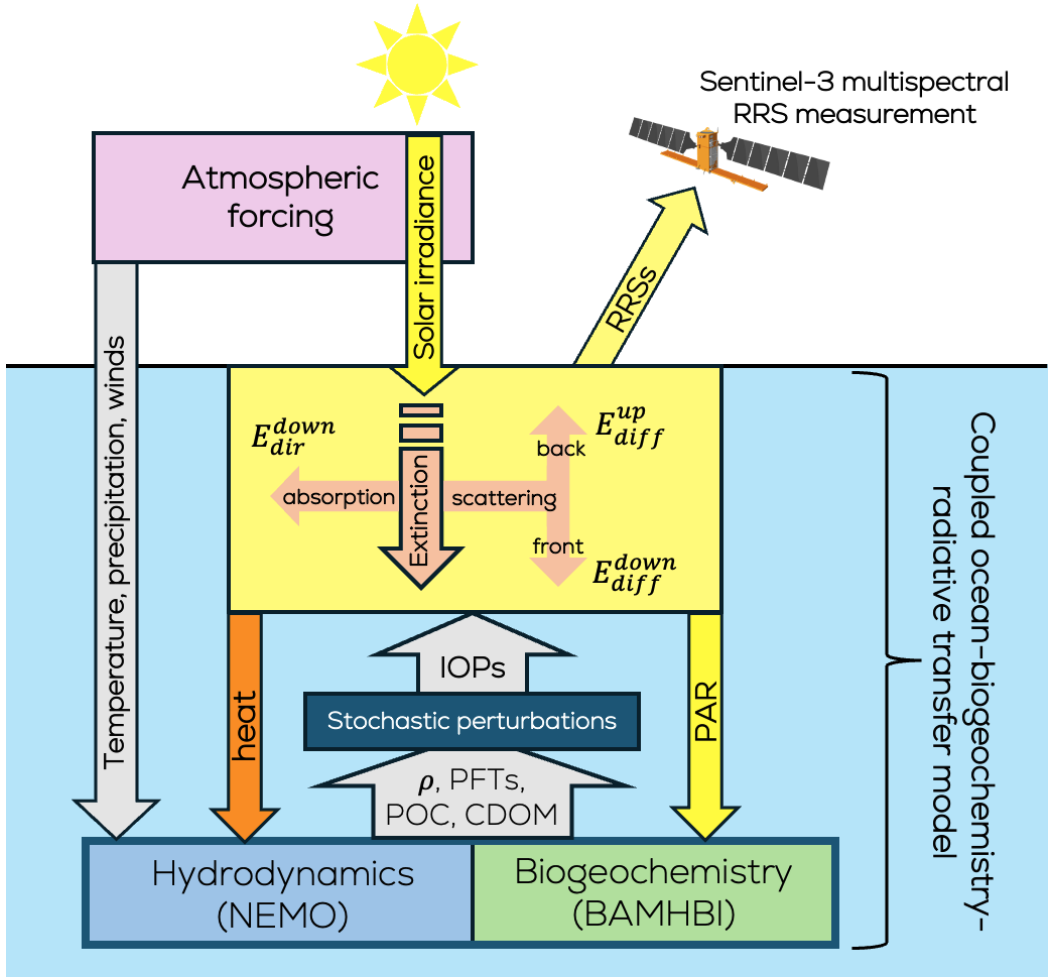
NWP precedent — moved from retrieved temperature/humidity profiles to raw satellite radiances in the 1990s; the operational skill gain was substantial and permanent *(Derber & Wu 1998; Weng 2007).*

OBSERVATION	PROCESSING	REFERENCE
Total chlorophyll	OC retrieval algorithm	*Natvik & Evensen 2003; Ciavatta 2011*
Plankton functional types	Spectral PFT retrieval	*Ciavatta 2018; Pradhan 2020*
Single-band R_{RS}(551)	Forward RT (single wavelength)	*Jones 2016 — Great Barrier Reef*
Multispectral R_{RS} (6 bands)	**Full forward RT, EnKF**	***This work — Black Sea***

Each step relaxes the compression of the spectral signal — the less preprocessing, the more constraint.

The coupled modelling framework

NEMO + BAMHBI + RADTRANS, two-way coupled



NEMO v4.2 — ocean physics (Black Sea, 15 km, 59 levels)

BAMHBI — biogeochemistry (28 pelagic + 6 benthic vars)

RADTRANS — 3-stream radiative transfer

Dutkiewicz 2015 / Macé et al. 2025a,b

MAR regional atmosphere with ecRad spectral SW

33 wavebands into RT (Grailet 2024)

Two-way coupling: RT produces both R_{RS} and sends PAR back into BGC

What the radiative transfer sees

the IOP decomposition tells us where corrections can and cannot land directly

$$\frac{dE_d(\lambda)}{dz} = -\frac{a(\lambda)+b(\lambda)}{\overline{\upsilon_d}}E_d(\lambda), \quad \text{x 3}$$

E_d – direct light
E_s – scattered downward light
E_u – backscattered light

$$R(\lambda) = \frac{E_u^{\text{below}}(\lambda)|_{k=0}}{E_{d_o}^{\text{below}}(\lambda) + E_{s_o}^{\text{below}}(\lambda)},$$

$$a(\lambda) = a_w(\lambda) + a_{phy}(\lambda) + a_{det}(\lambda) + a_{cdom}(\lambda),$$
$$b(\lambda) = b_w(\lambda) + b_{phy}(\lambda) + b_{det}(\lambda),$$
$$b_b(\lambda) = b_{bw}(\lambda) + b_{bphy}(\lambda) + b_{bdet}(\lambda).$$

$(a, b, b_b)_w$
Pure water absorption, scattering and backscaterring

$(a, b, b_b)_{phy}$
3 phytoplankton groups absorption, scattering and backscaterring

$(a, b, b_b)_{det}$
POC absorption, scattering and backscaterring

a_{CDOM}
Colored dissolved organic matter absorption (parametrized)

BAMHBI provides:

- **Carbon in phytoplankton**
- **CHLa in phytoplankton**
- **POC concentration**

What this predicts for DA?

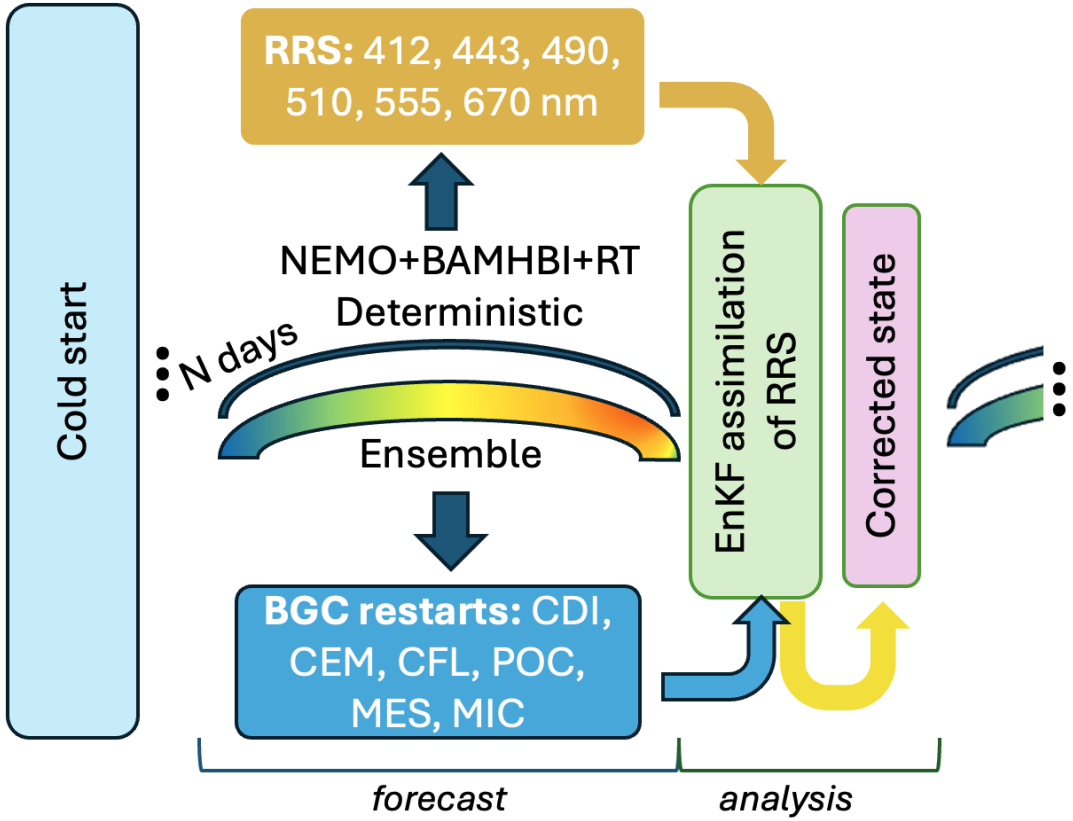
CPHY + POC
directly in RT — state vector corrects via inversion of forward model

CDOM
parameterised, not prognostic → mismatch becomes a diagnostic signature (slide 11)

Zooplankton
outside RT equations → corrected through ensemble covariance + trophic coupling

Assimilation setup

six-channel R_{RS} assimilated through the forward RT operator — no inversion



Observation: R_{RS} at 412, 443, 490, 510, 555, 670 nm

Observation operator: the RT solver itself

State vector: CDI, CEM, CFL, POC, MIC, MES

(phytoplankton + particulate + zooplankton)

Ensemble: 20 members, stochastic IOP perturbations

Macé et al. 2025a

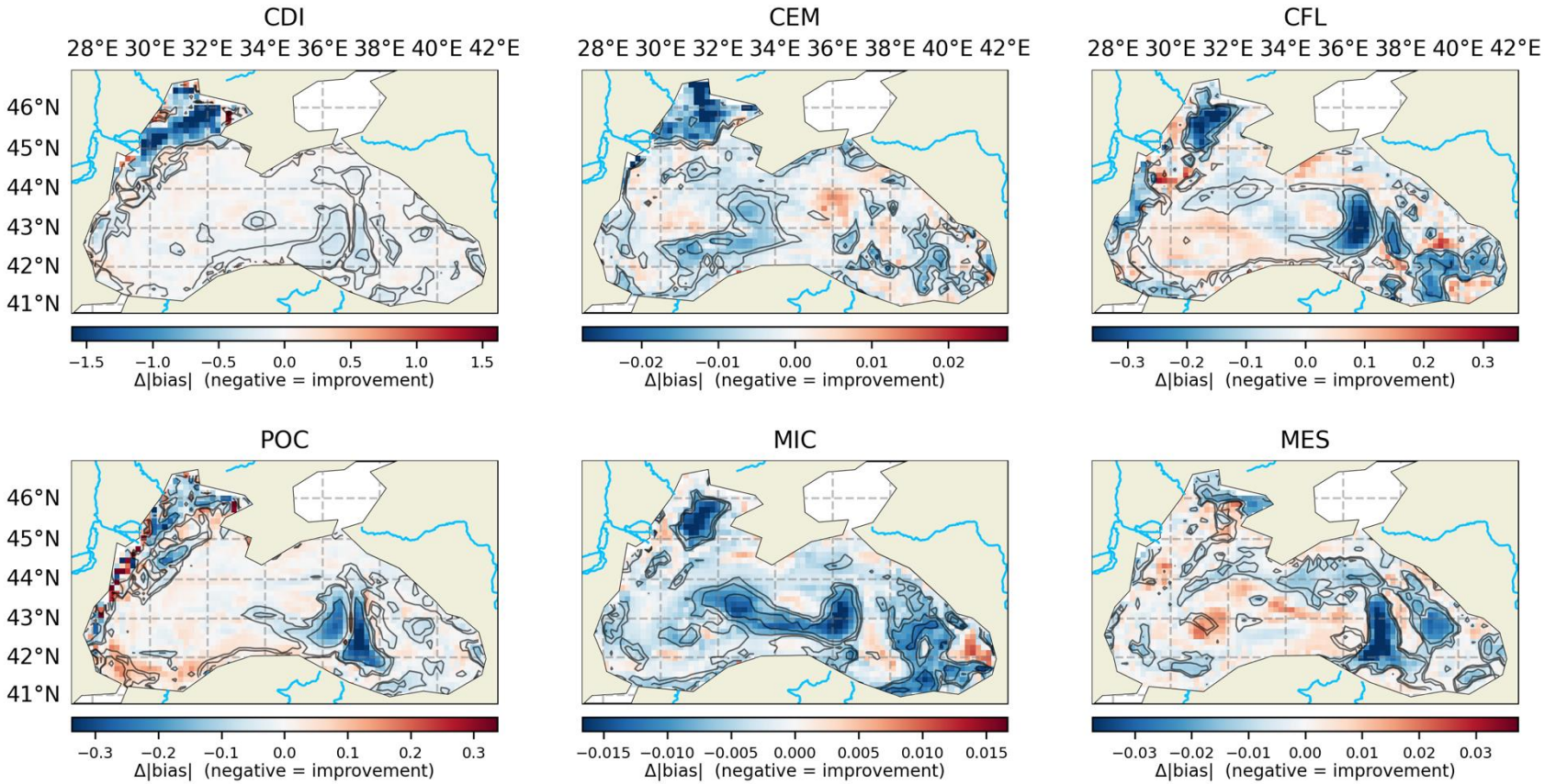
Filter: ETKF (OAK), daily cycle, RTPS α = 1

OSSE: brother-twin — deterministic run = synthetic obs

Covariance propagation: *the ensemble covariance applies increments across all 59 vertical levels*

All six state variables improve

annual bias improvement maps — blue indicates reduction of error



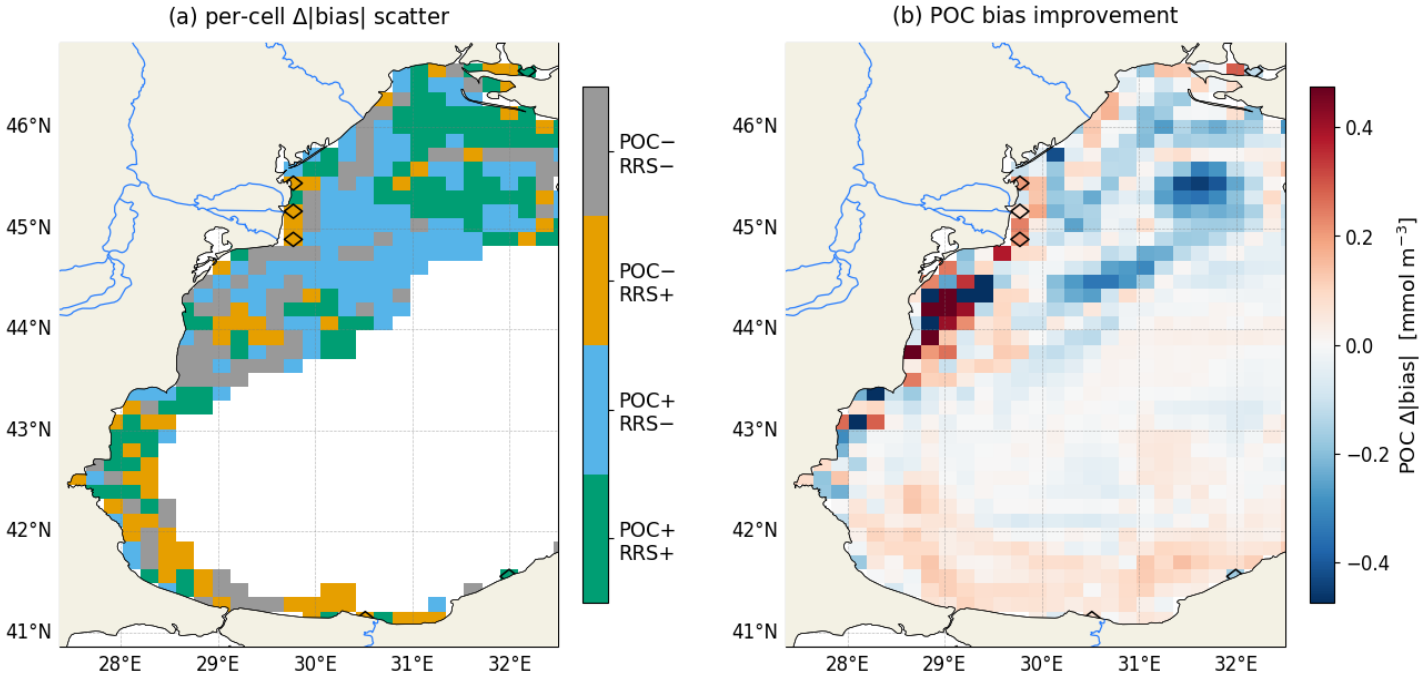
|bias| improvement, shelf / deep basin:

	shelf	deep
CDI	46%	46%
CEM	68%	57%
CFL	55%	55%
POC	49%	30%
MIC	58%	72%
MES	26%	66%

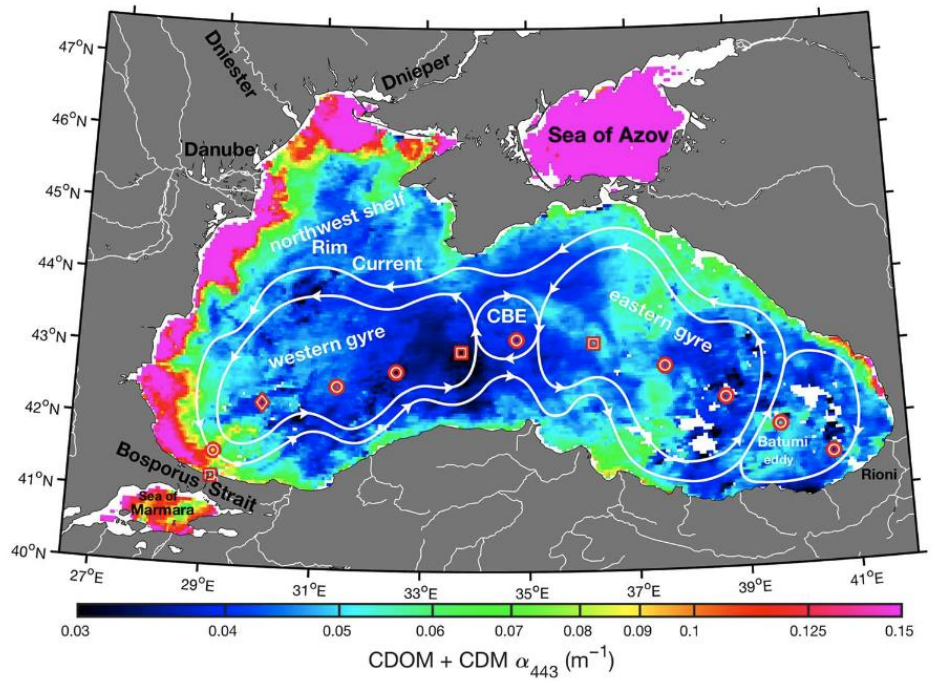
Zooplankton (MIC, MES) corrected despite no direct optical signature — ensemble covariance + trophic coupling, as predicted by the IOP structure (slide 5).

CDOM as a diagnostic probe

the compensatory POC signature maps the independently observed CDOM distribution



Quadrant classification of each shelf grid cell based on the sign of Δ|bias| for RRS(443) and depth-weighted POC

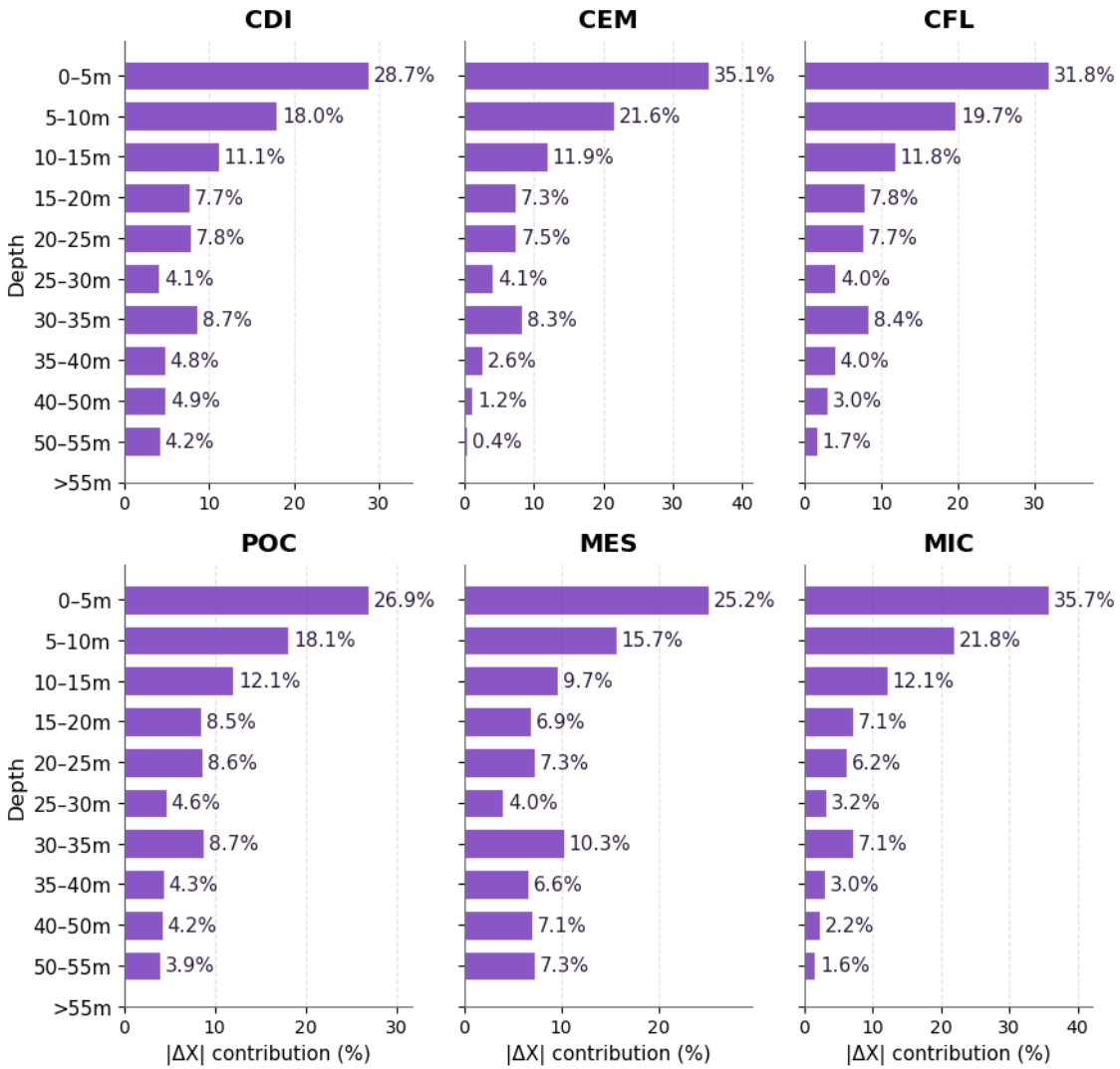


(c) satellite CDOM climatology — Margolin et al. 2018

Reflectance assimilation does not just correct — *it highlights priority direction of the Black Sea biogeochemical-optical model development*

Vertical propagation

surface R_{RS} → ensemble covariance → corrections at all depths



Corrections not confined to the surface

— covariance distributes them across the water column.

Peak increment at 30–35 m

— across all 6 state variables.

This depth coincides with the climatological DCM

position in the Black Sea (Ricour 2021).

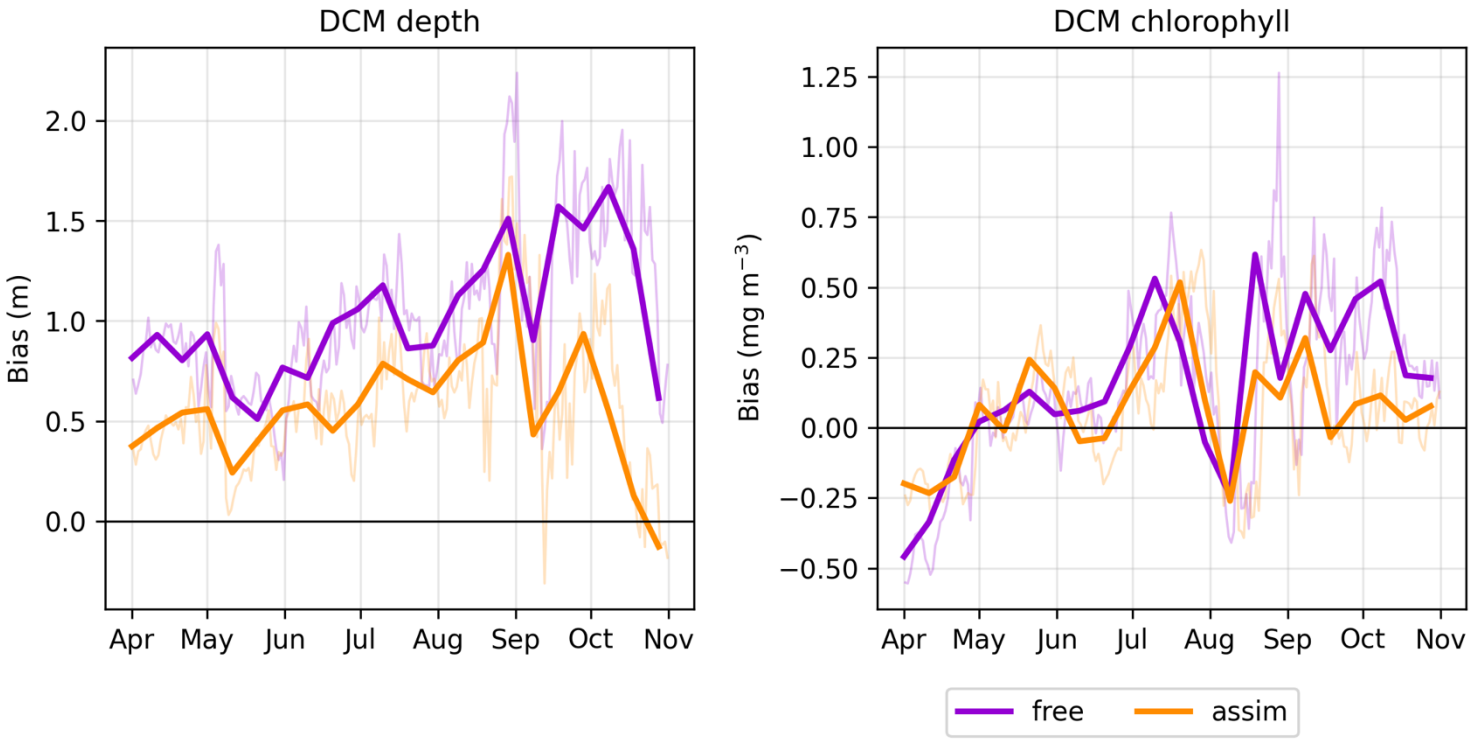
This is the bridge: can we show it also improves the DCM itself?

Vertical distribution of assimilation increments: for each variable, the share (%) of total |ΔX| falling in each depth bin, averaged over the basin and the 2016 assimilation period.

The DCM responds

Strict detection (Ricour et al. 2021) · Apr–Nov stratified season · daily basin-mean bias

Deep Chlorophyll Maximum (DCM): *a subsurface biomass peak forming where light and nutrients balance. In the Black Sea, typically at 25–35 m during stratification (Ricour 2021).*



Teruzzi et al. 2021

(Mediterranean, 3DVar, OC + in-situ profiles) reports comparable 13–20% subsurface chlorophyll RMSD reduction, without a reported depth bias.

DCM depth

44%

|bias| 1 → 0.52 m

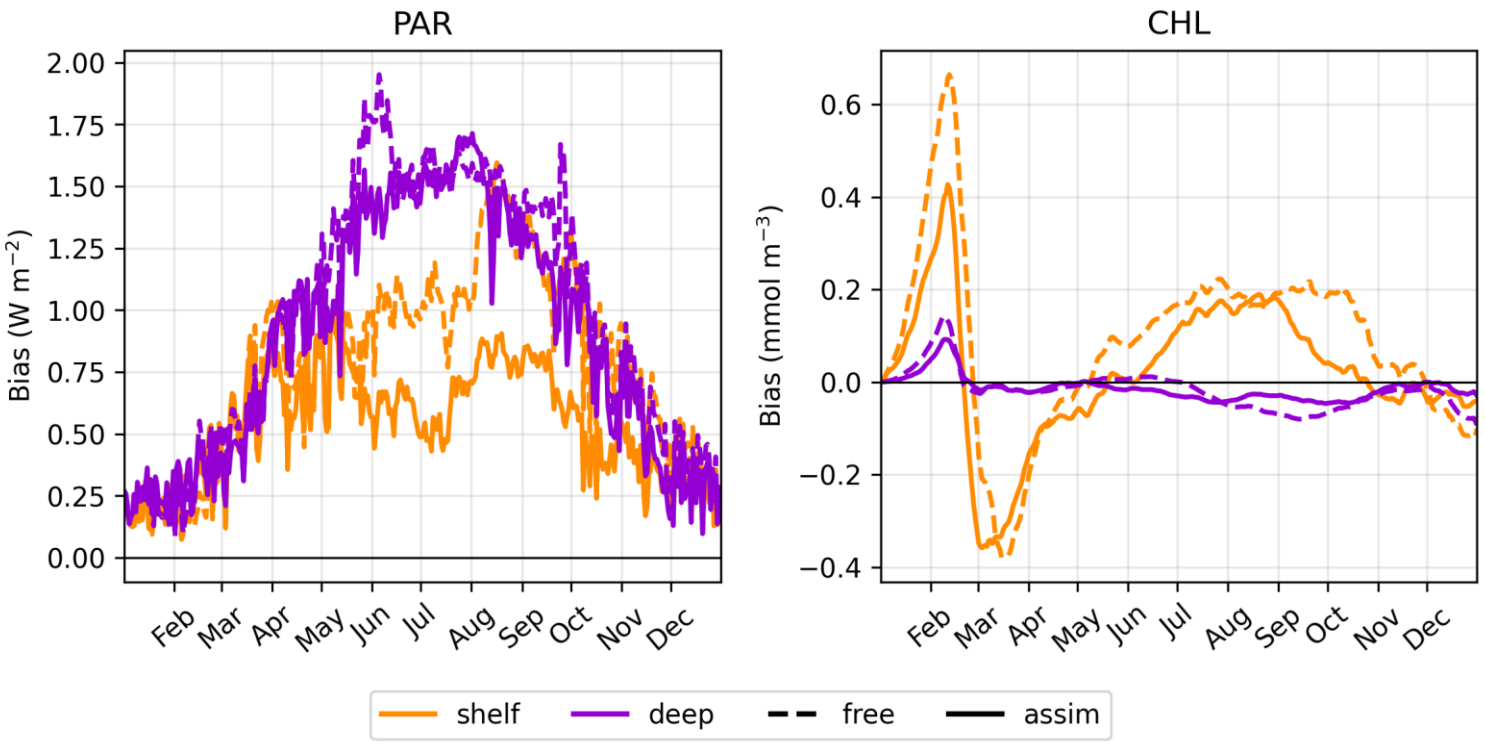
DCM CHL intensity (RMSE)

22%

RMSE 1.19 → 0.93 mmol m⁻³

The light field follows

PAR is not assimilated — corrected via the two-way RT coupling



Chain of correction

CPHY carbon correction

↓

diagnostic chlorophyll field

↓

water-column attenuation

↓

PAR response

	|bias|	CRPS
CHL	31%	41–44%
PAR shelf	30%	28%
PAR deep	8%	11%

Take-aways

what this study establishes — and what it does not

1 3D ecosystem constrained from surface

Surface multispectral R_RS constrains the full three-dimensional chlorophyll field via covariance propagation.

2 The DCM is reached

Depth (44%), width (52%) and intensity (22% RMSE) all corrected — through surface observations alone, comparable to in-situ-assisted schemes.

3 Light field follows via two-way coupling

PAR is corrected (30% shelf) despite being outside the state vector — through RT ↔ BGC coupling.

4 Diagnostic probe for model deficiencies

Compensatory POC signature maps independently observed CDOM — works as a model deficiencies diagnostic.

Honest limits. *Brother-twin OSSE suppresses structural errors shared between twin and ensemble. Magnitudes are mechanism demonstration — real-data verification is the next step.*

Where this goes next

the OSSE is the start — real data and model development are next

Next steps

Real-data application: Sentinel-3 OLCI, PACE hyperspectral

Make CDOM prognostic in BAMHBI

+ shelf-targeted sampling (gliders, moorings)

Add Emiliana calcification in BAMHBI

Higher resolution (15 → ~5 km) for coastal processes

ML parameter estimation complementing EnKF state correction

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Thank you

Questions welcome.

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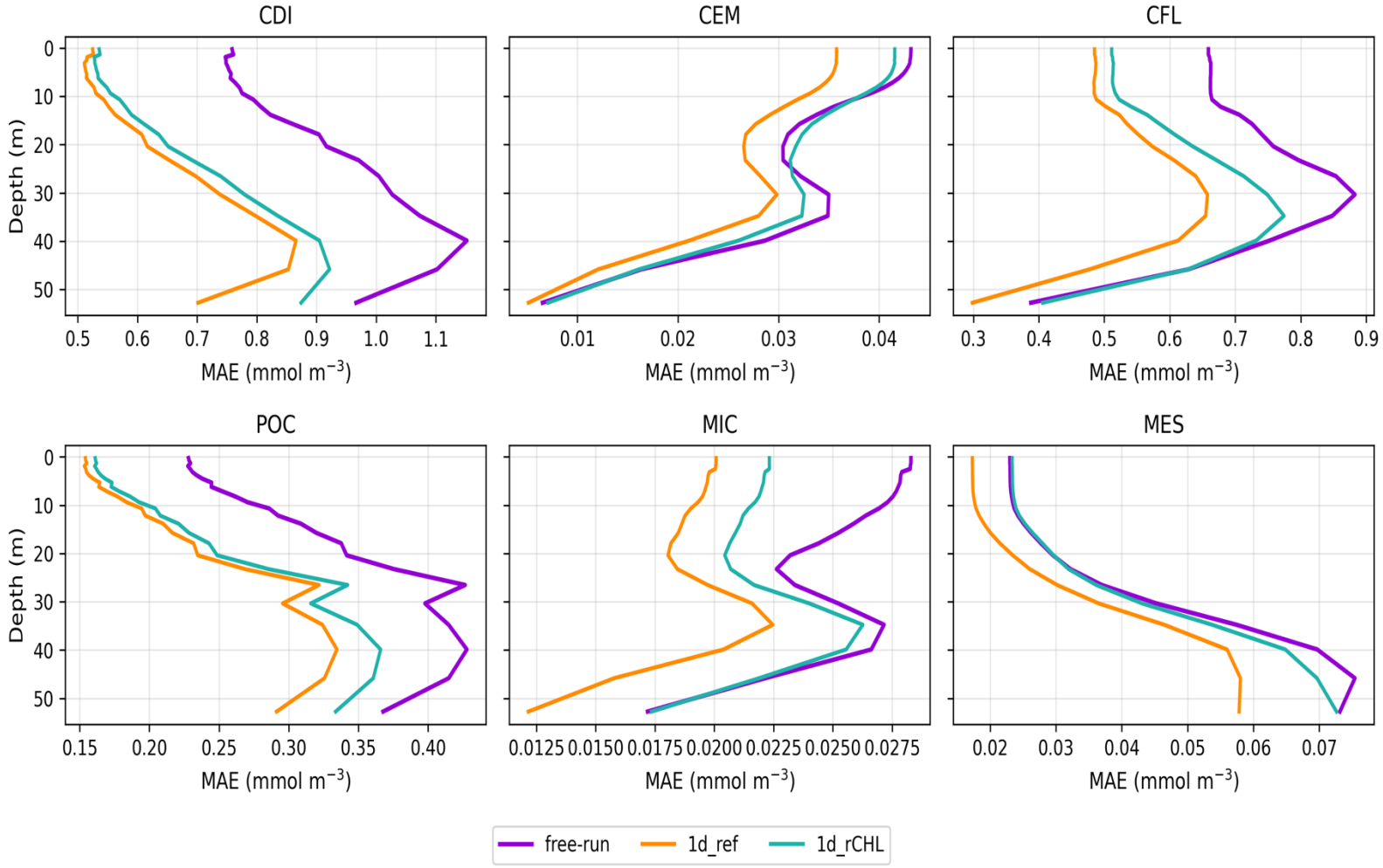
The full Satellite Ocean Reflectance Data Assimilation (SORDA) framework implementation and coupled NEMO-BAMHBI-RT model configuration are published on the MAST GitLab page: https://gitlab.uliege.be/especes/mast/SORDA

SORDA offline version was delivered as a NECCTON WP4 deliverable: https://github.com/neccton-algo/SORDA

BONUS

Multispectral vs derived chlorophyll

same framework, two observations: six-band R_{RS} vs Kajiyama B/R chlorophyll



Three patterns

Regional — multispectral advantage grows in CDOM-rich waters; rCHL degrades 4/6 vars in deep basin.

Variable — largest gap for POC, MIC, MES (no direct chl signature). Shelf MES: multispectral +26%, rCHL −47%.

Temporal — multispectral maintains skill outside bloom; rCHL converges to free run (July onwards).