PDAF Parallel Data Assimilation Framework

Coupled assimilation of satellite temperature and chlorophyll observations for improved ecosystem predictions in the Baltic Sea

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SEAMLESS

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Model: NEMO-NORDIC

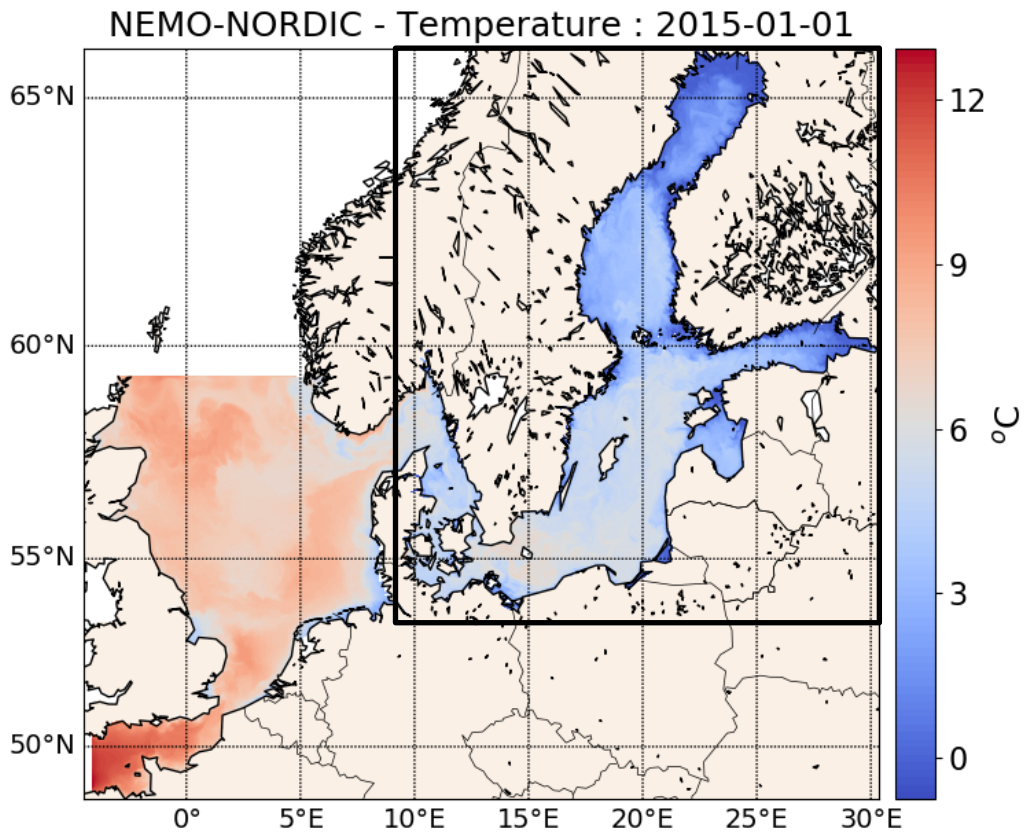
Operational configuration of European Copernicus Baltic Monitoring and Forecasting Center (BAL-MFC)

Model setup

- NEMO-NORDIC
- 1 nm resolution (~1.8km, ~1000x1200 grid points)
- 56 layers
- Time step 90 sec
- Open boundaries in North Sea and English Channel
  - BCs from separate model for North Atlantic

Operational use in CMEMS BAL-MFC

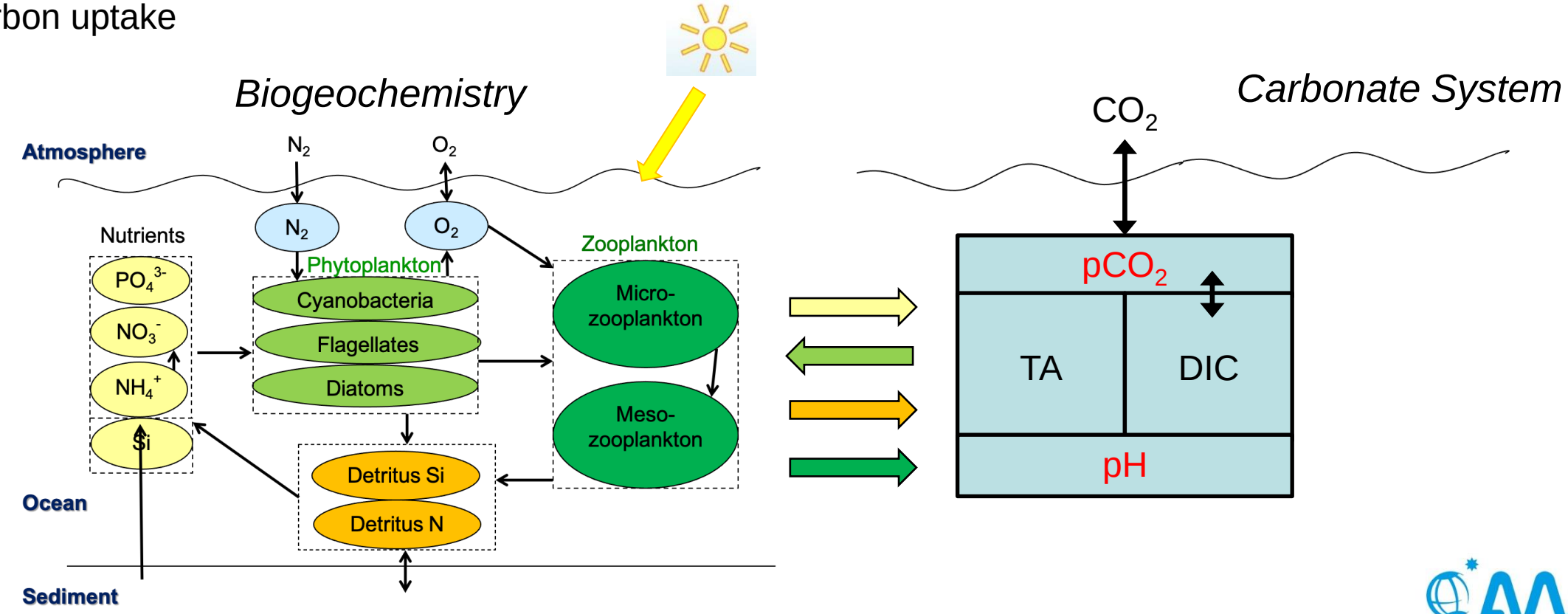
- Assimilation with PDAF in offline mode
- Near-real time and multi-year products
- 'blue ocean' (physics)
  - assimilation of surface temperature
- 'green ocean' (Ecosystem, water quality)
  - Assimilation of nitrogen and oxygen profiles



BGC Model: ERGOM

- original development for Baltic Sea (Neumann, 2000)
- based on nitrogen
- module for carbonate system was recently added
- Applications, e.g.
  - Water quality (nutrification, algal blooms, oxygen deficit zones)
  - Carbon uptake

For data assimilation
- 20 model variables (16 prognostic, 4 diagnostic)
- Observed chlorophyll is diagnostic variable



PDAF – Parallel Data Assimilation Framework

PDAF Parallel Data Assimilation Framework

A unified tool for interdisciplinary data assimilation …

- provide support for parallel ensemble forecasts
- provide DA methods (EnKFs, smoothers, PFs, 3D-Var) - fully-implemented & parallelized
- provide tools for observation handling and for diagnostics
- easily useable with (probably) any numerical model
- a program library (PDAF-core) plus additional functions
- run from notebooks to supercomputers (Fortran, MPI & OpenMP)
- ensure separation of concerns (model – DA method – observations – covariances)
- first release in year 2004; continuous further development

Open source:
Code, documentation, and tutorial available at

https://pdaf.awi.de

github.com/PDAF

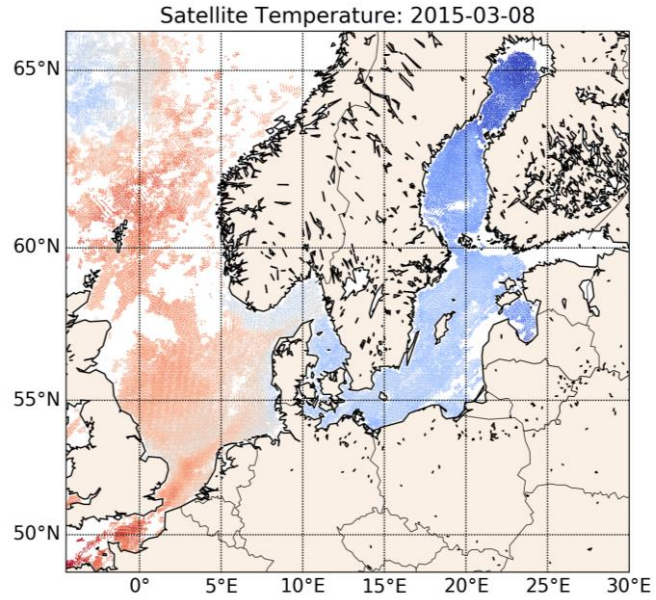
L. Nerger, W. Hiller, Computers & Geosciences 55 (2013) 110-118

AWI

Observations

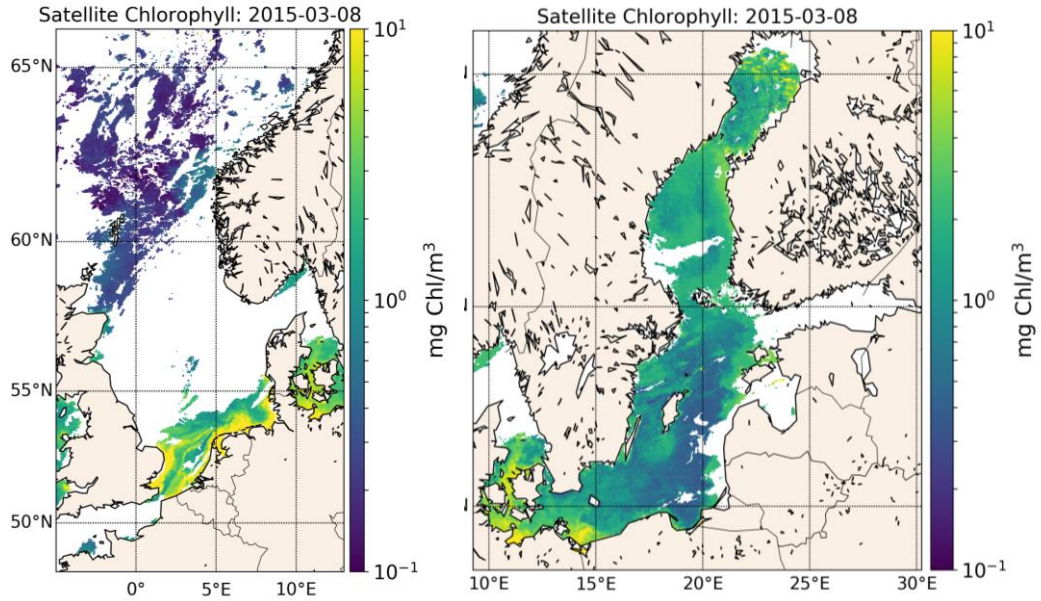
Sea Surface Temperature (*SST*)

- Level 3 data from CMEMS
- resolution 0.02º
- available daily
- observation error for DA: 0.8 ºC
  (provided error fields not fully realistic)



Chlorophyll (*CHL*)

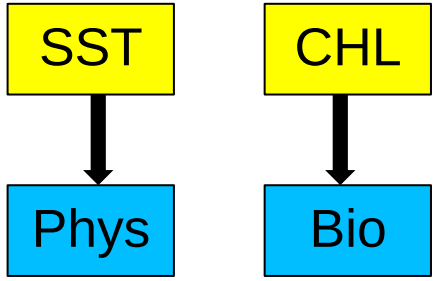
- Level 3 data from CMEMS (multi-satellite multi-year)
- separate data products for North Sea and Baltic Sea
- resolution 1 km
- available daily
- observation error: relative error of 0.3
- Coverage worse than SST



Weakly and Strongly Coupled Data Assimilation

Weakly coupled DA (CHLw+SSTw)

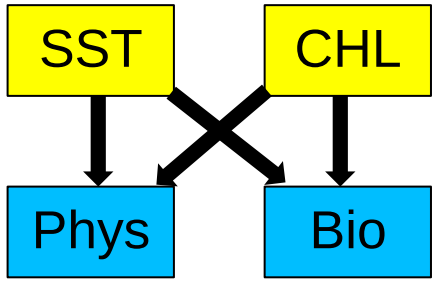
- Assimilate SST observations only into physics
- Assimilate chlorophyll (CHL) observations only into ERGOM



Strongly coupled DA (CHLs+SSTs)

- Update both physics and ERGOM using both observation types

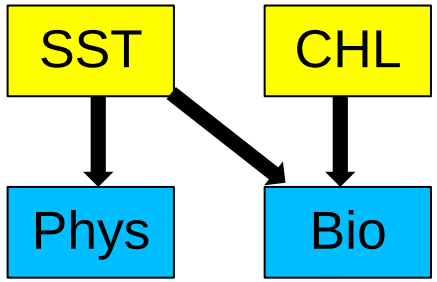
  → *Improves ERGOM but leads to increased errors of temperature (error level of ERGOM and CHL data higher than NEMO & SST)*



Partly strongly coupled DA (CHLw+SSTs)

- Use SST observations to update physics and ERGOM
- Use CHL observations to update ERGOM

  → *Best results*



Data Assimilation Setup

Online-coupled DA system

- Augmented NEMO-ERGOM with DA functionality
- No model restarts required to apply DA

Ensemble States

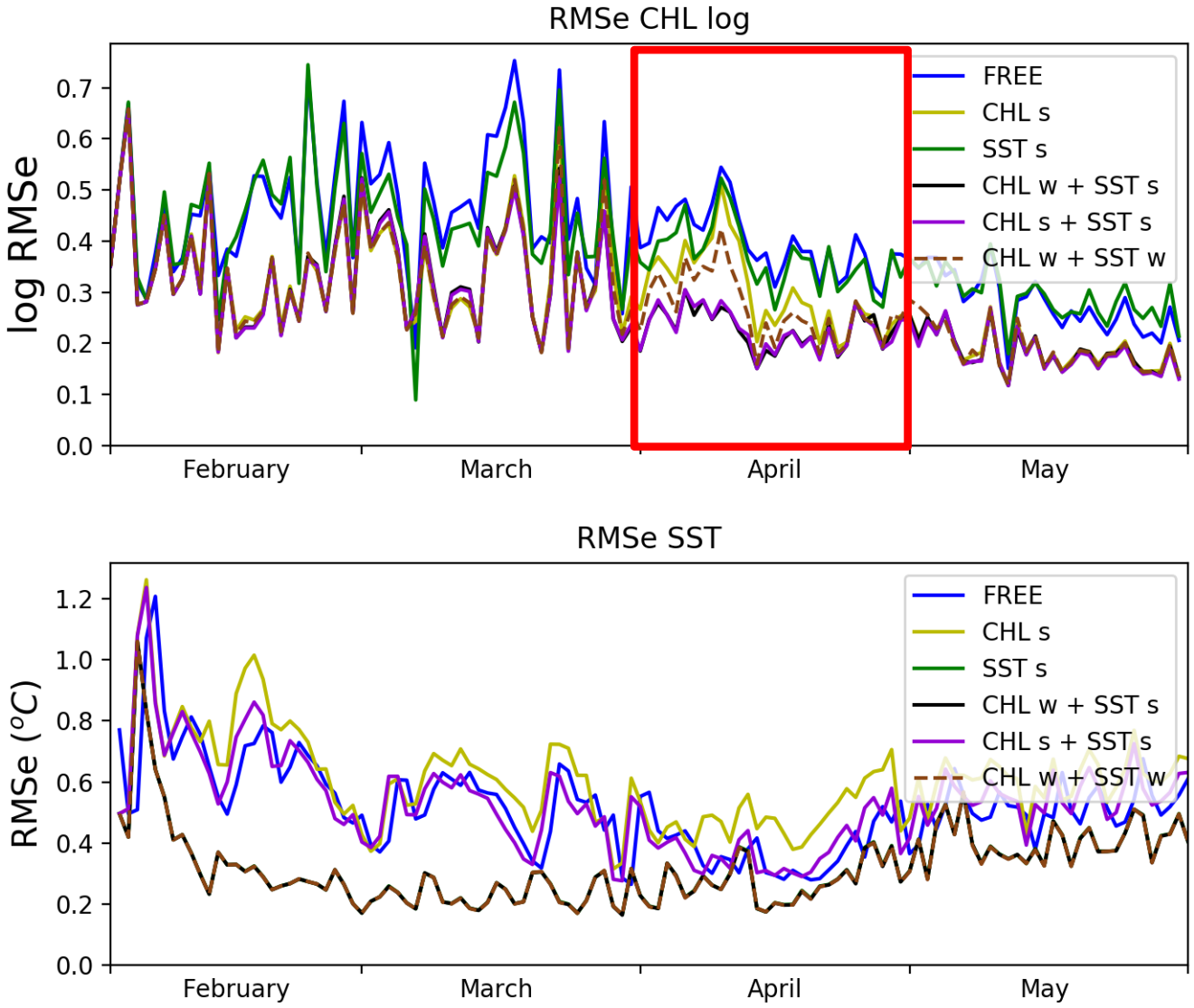
- 5 physics variables
- 16 ERGOM prognostic variables + 4 diagnostic variables
- State dimension: $704 \cdot 10^6$

Assimilation setup

- ensemble Kalman filter LESTKF
- ensemble size: 30
- Daily assimilation from February 1st

- *NEMO:* only 3D temperature updated
  (multivariate updates result in unrealistic salinity; 'feature' of NEMO)
- *ERGOM:* update 13 prognostic + 4 diagnostic variables
  (no update of LDON, DIC, ALK)

Effects of Assimilation – Baltic Sea (RMS errors)



Chlorophyll

- Assimilating only SST insufficient to constrain CHL
- Significant differences during April (reason not yet clear)

→ **CHLw+SSTs yields best result for both SST and CHL**

Temperature

- Strongly coupled DA of CHL deteriorates temperature (the run is stable…)

Forecasting: Initialized from DA

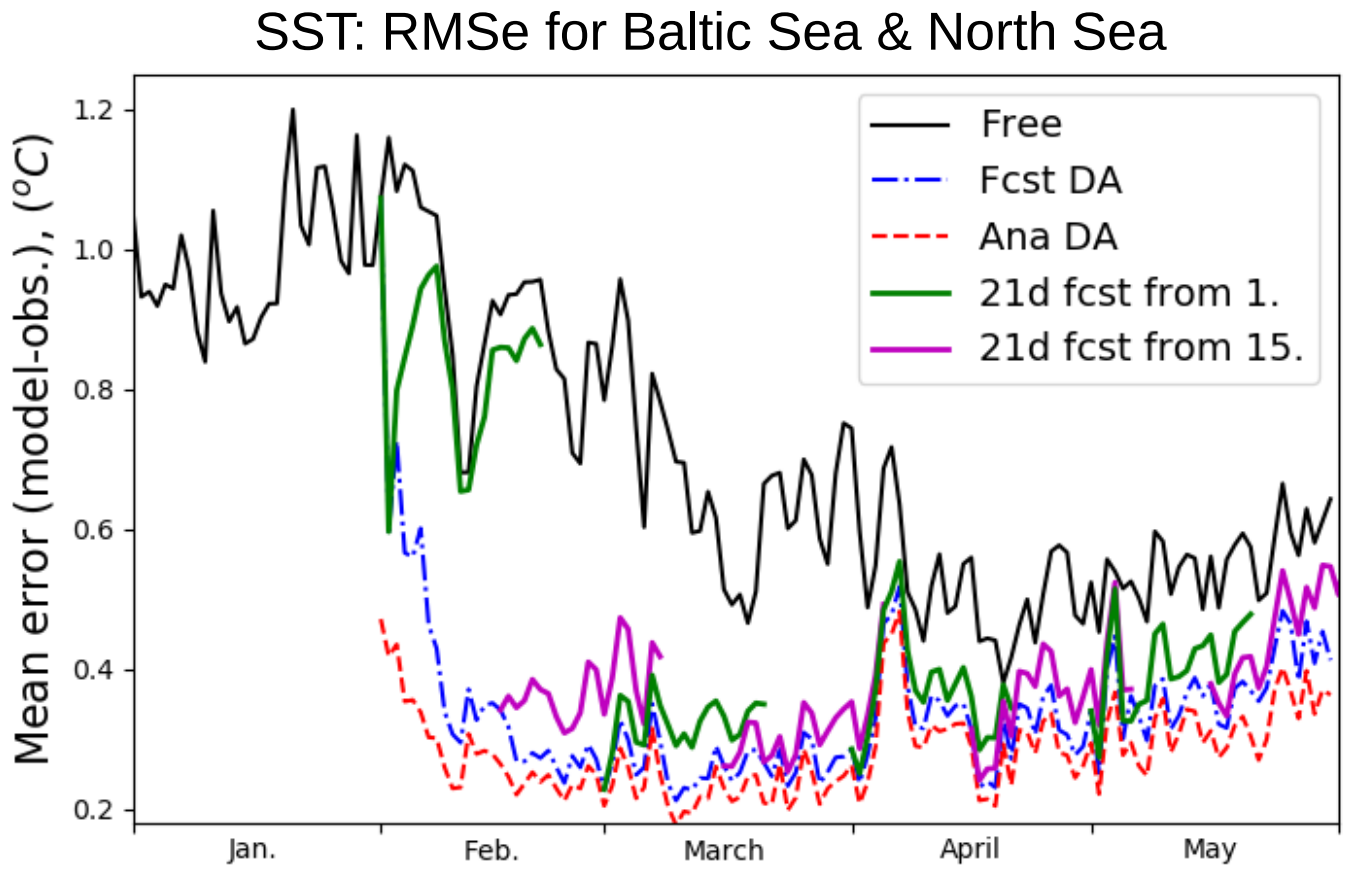
Ensemble run from Jan. 1, 2015

- ensemble perturbations in physics from EOFs (2nd-order exact sampling)
- ensemble central state from forecast
- perturb 15 process parameters of ERGOM

Data assimilation from Feb. 1, 2015

21-day forecasts

- Green: Initialized 1st of month
- Magenta: Initialized 15th of month
  - Slow error increases



DA: Effect on Chlorophyll

Daily assimilation from Feb. 1, 2015

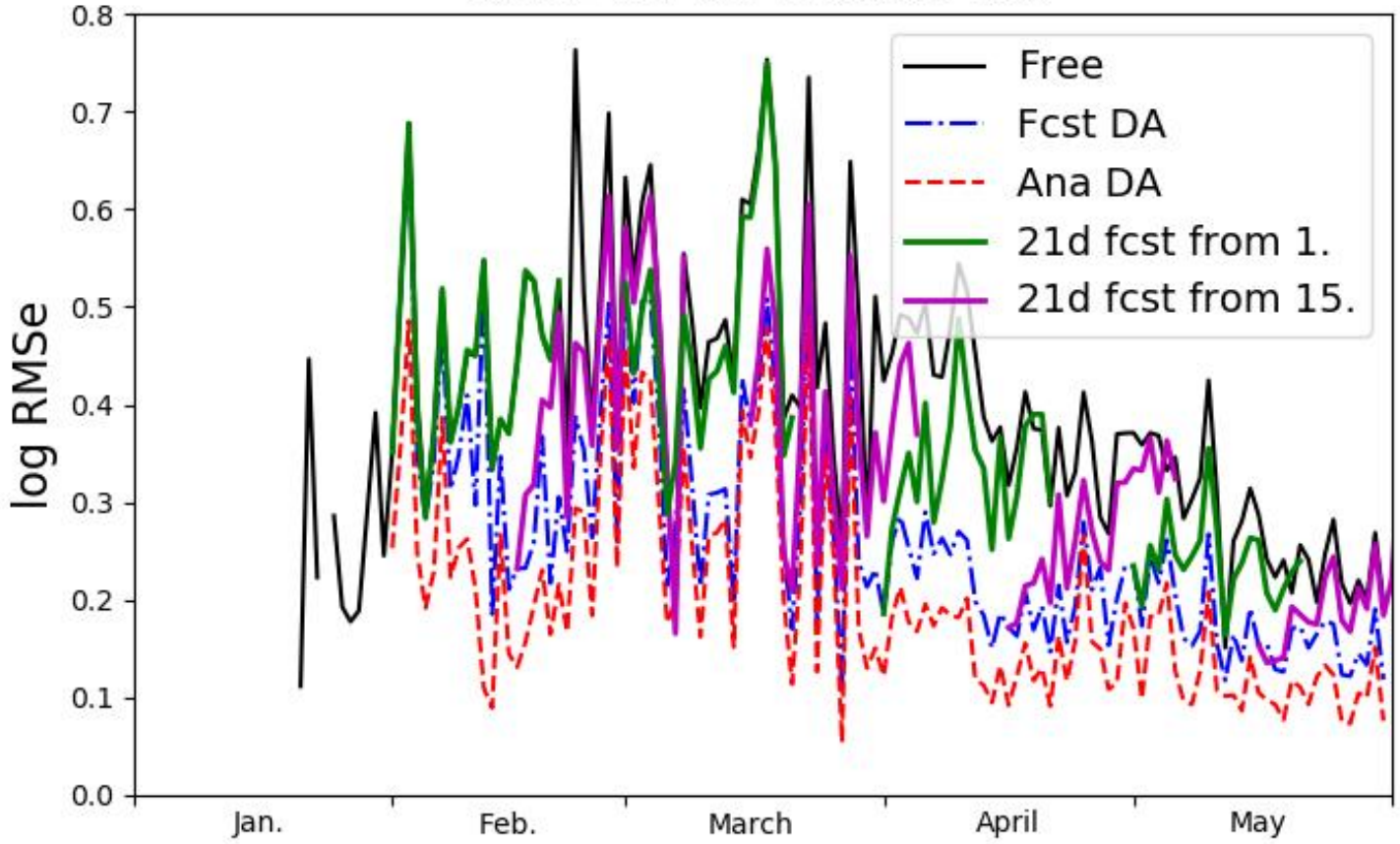
- Log-RMSe reduced
- Strong fluctuations in February and March (varying data coverage)

21-day forecasts

- Green: Initialized 1st of month
- Magenta: Initialized 15th of month

- Larger error increase than for SST (lower forecast skill)

Chlorophyll: Log10-RMSe in Baltic Sea



Effect of DA on longer forecasts: Chlorophyll

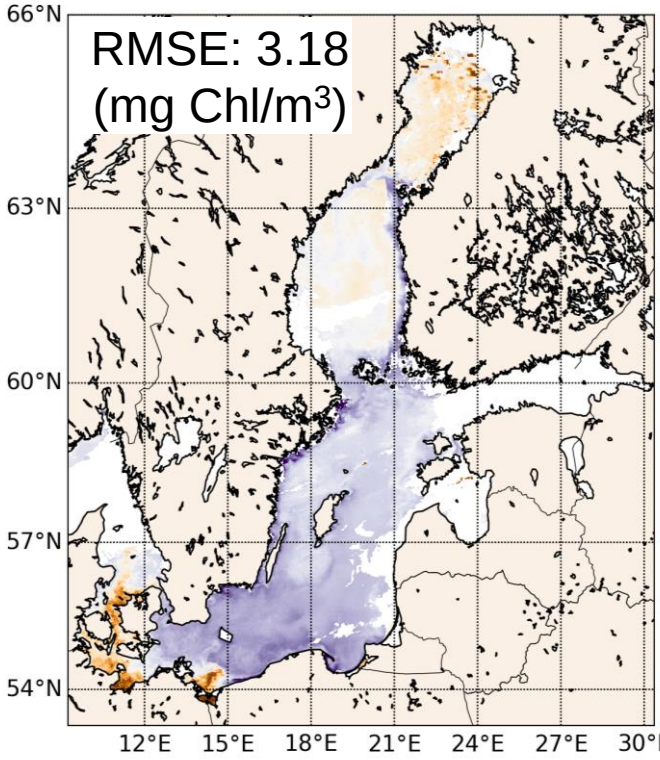
Performed 14-day ensemble forecasts initialized from DA analysis

- Error reduction in 24-h forecast: 33 %
  8-day forecast: 20 %
  14-day forecast: 5 %

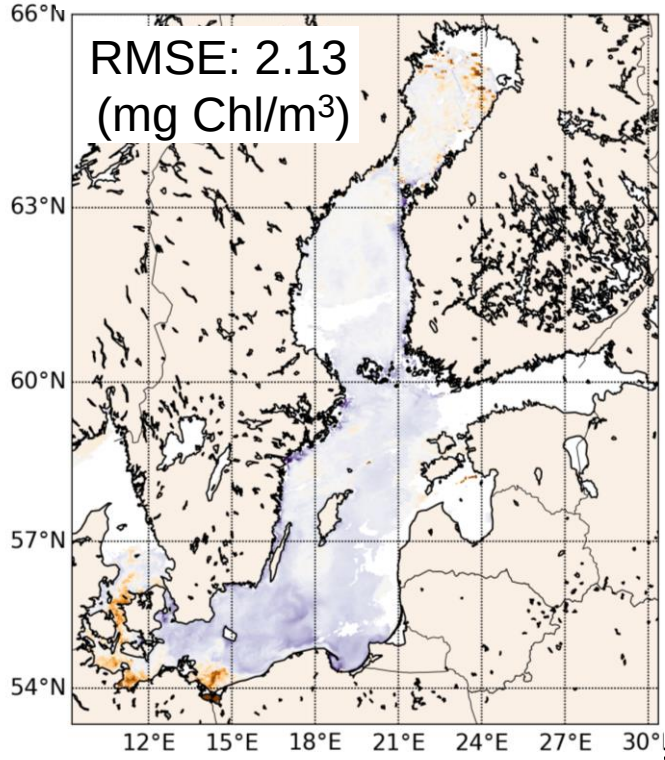
Faster error increase for biogeochemistry than physics
➜ caused by biases

Surface chlorophyll: model - observations

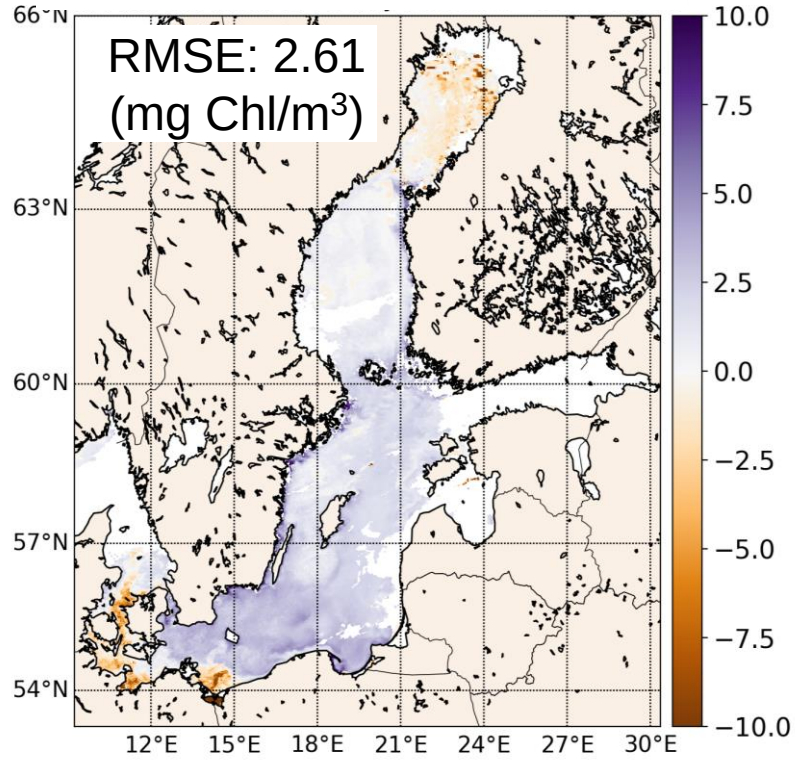
Free run on March 9



24h forecast (init March 8)



8-day forecast (init March 1)



Effect of DA on Ecosystem Indicators

SEAMLESS project selected several ecosystem indicators

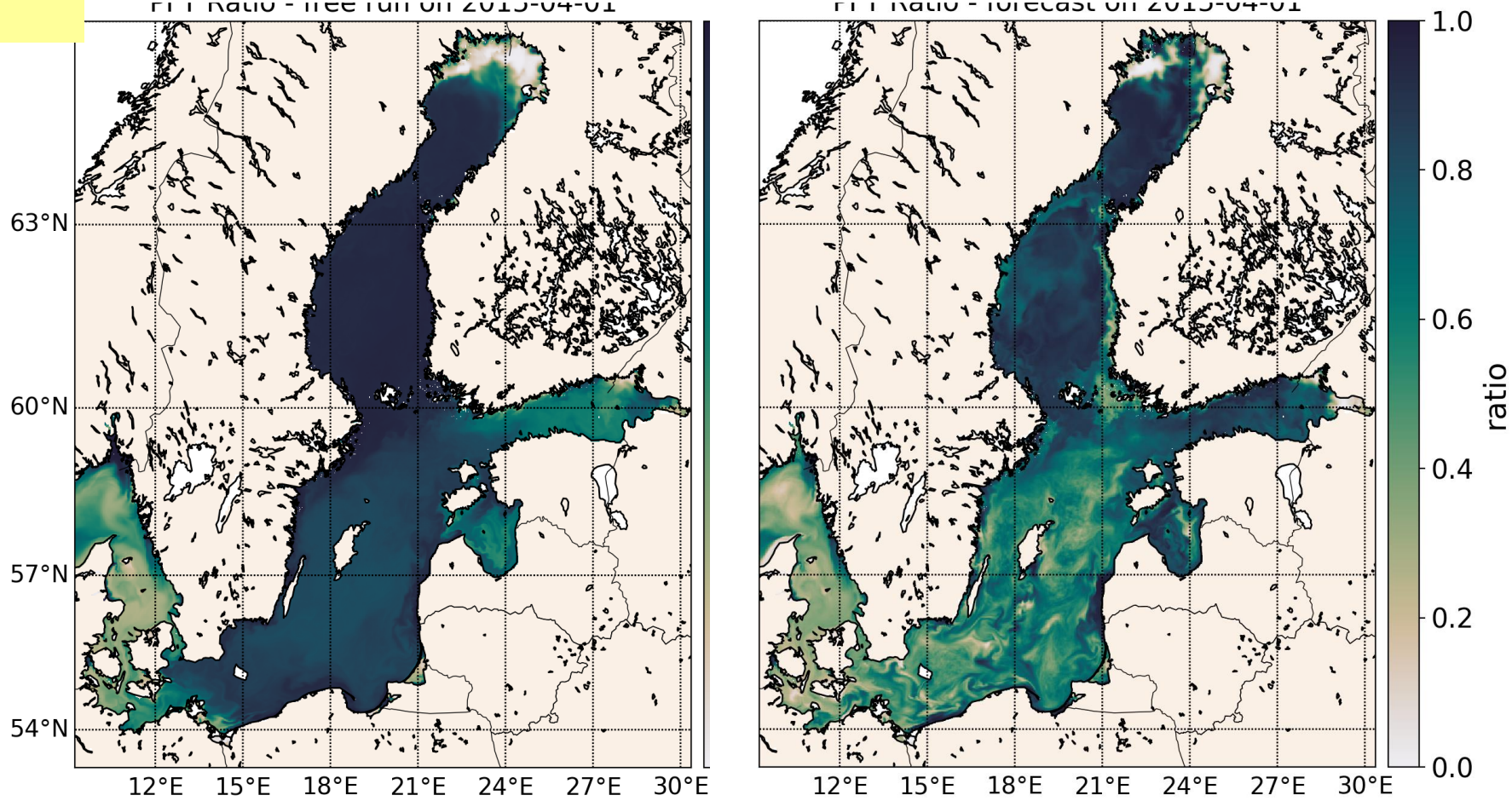
Ratio of diatoms to total phytoplankton

DA reduces relative abundance of diatoms in several regions

(difficult to validate)

Free run on April 1

24h forecast on April 1



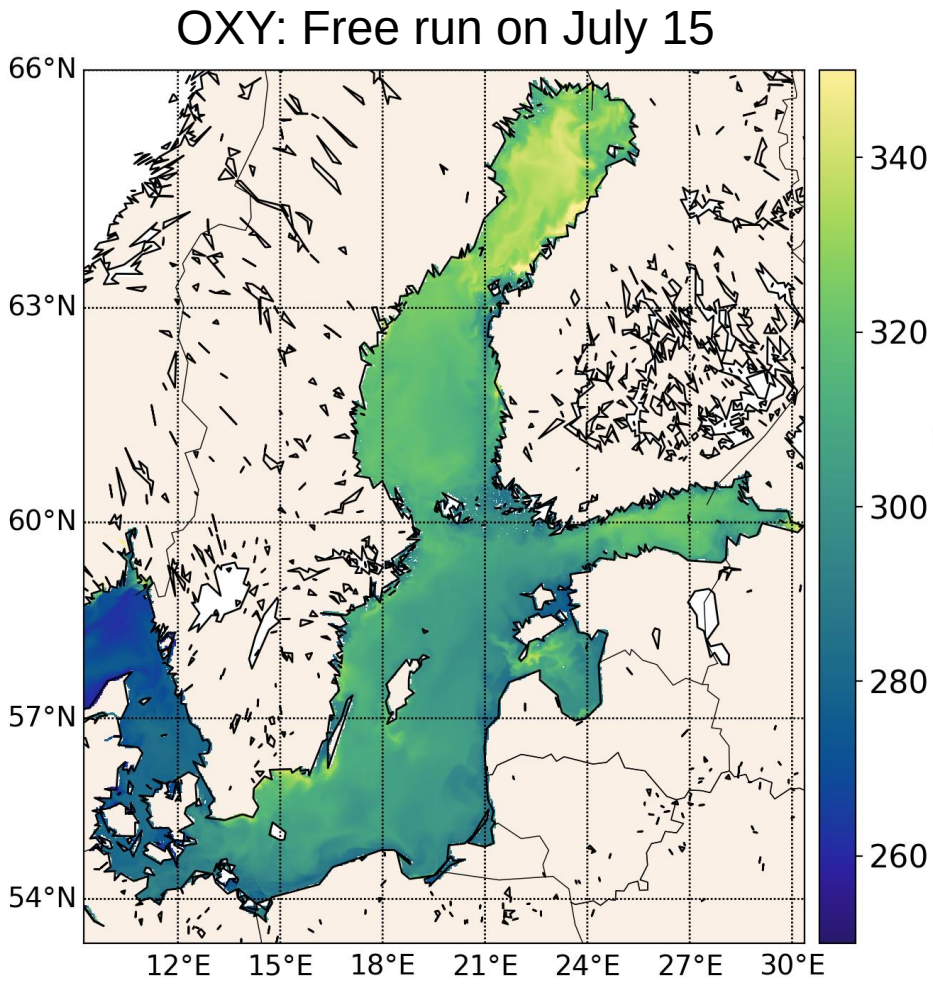
Effect of DA on Ecosystem Indicators

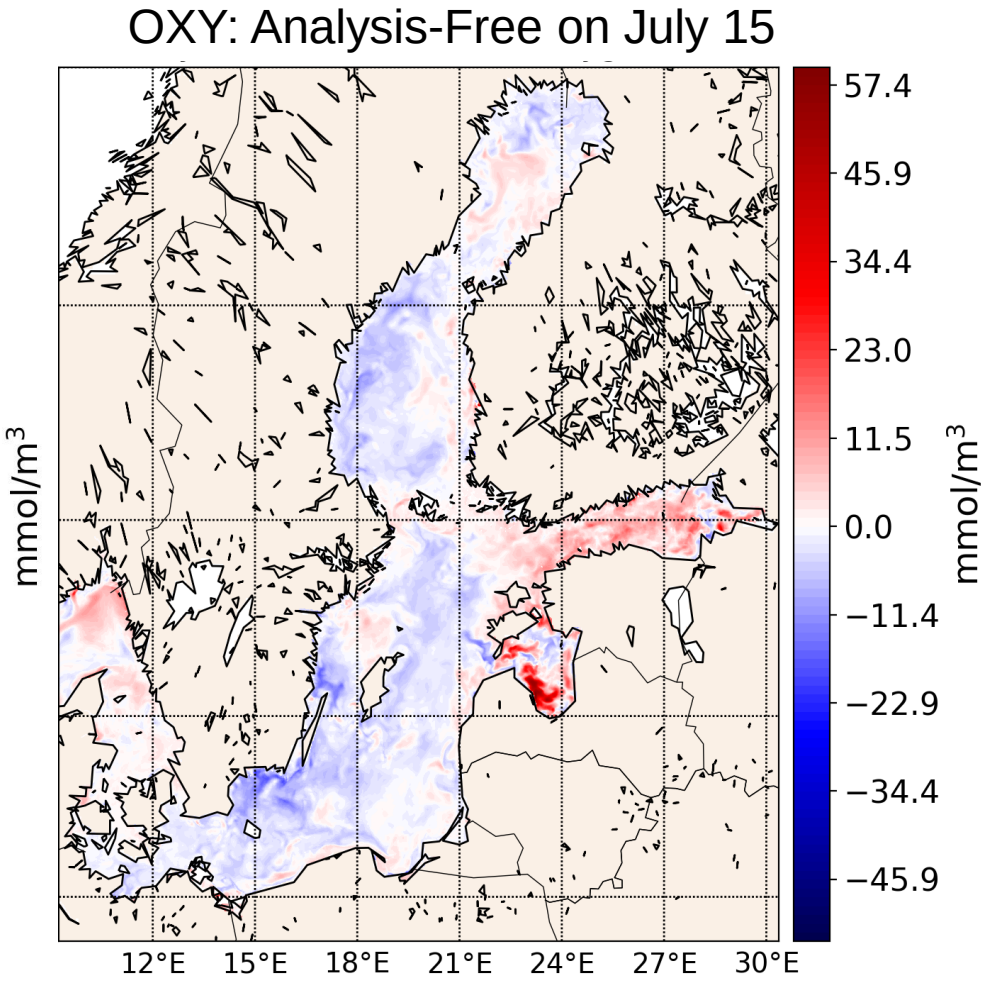
Oxygen

DA increases concentrations in Gulfs of Finland and Riga (eastern Baltic), lower conc. In most regions

Oxygen is not sufficiently constrained from SST and CHL data

➜ need oxygen insitu data





Summary

PDAF Parallel Data Assimilation Framework

- Coupled assimilation of satellite SST and chlorophyll using PDAF enhancing the currently used operational forecasting system
- Improvements in temperature and chlorophyll in analysis and forecasts up to 21 days
- System allows predictions of the ecosystem state and derived indicators
- Combined SST+CHL assimilation improves result over CHL-only assimilation (best is combined weakly-strongly coupled assimilation)

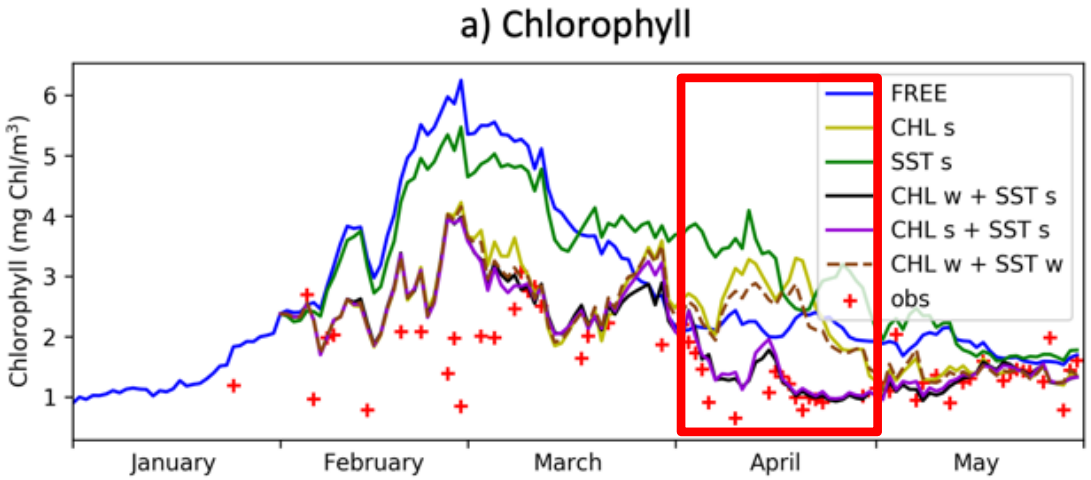
Open developments and inter-operability

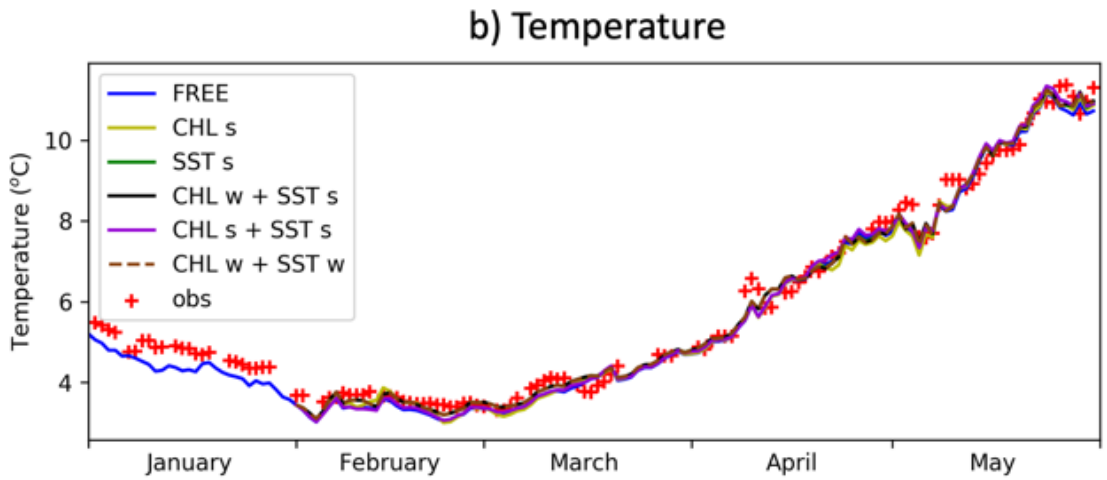
- **PDAF** is model agnostic, open source & ensures separation of concerns (pdaf.awi.de, github.com/PDAF/PDAF)
- **NEMO-PDAF** coupled is available open source (github.com/PDAF/NEMO-PDAF)
- Code developments can easily be adapted to other models or configurations (e.g. for digital twins and machine learning)

NEMO-PDAF
See Poster today

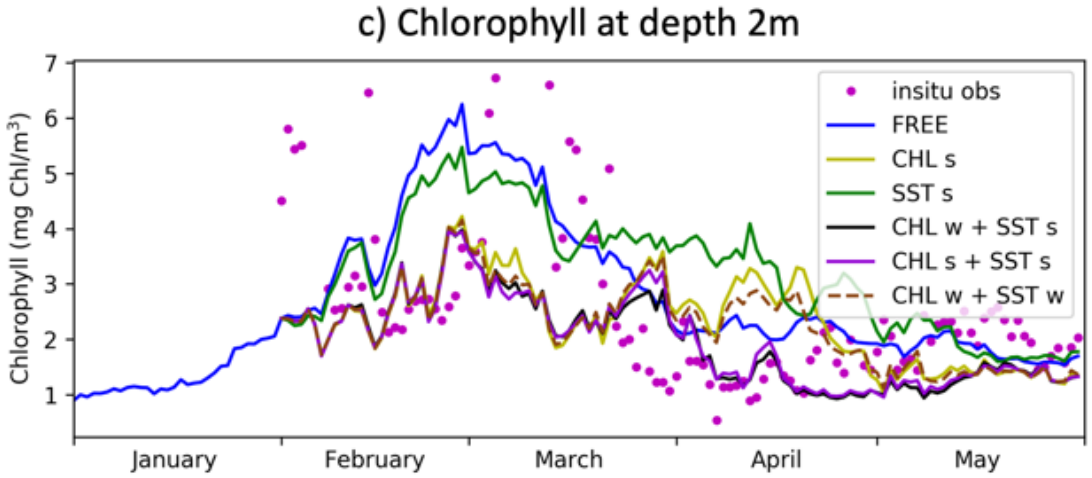
Effects at Station Darss Sill (southern Baltic) – actual values

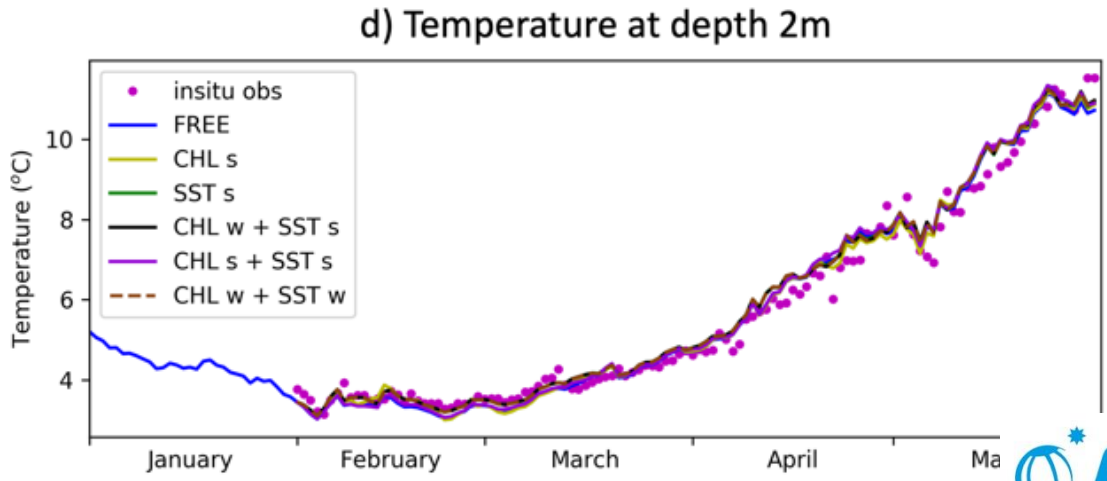
Comparison to assimilated satellite data





Comparison to independent in situ data





PDAF – Unified tool for interdisciplinary data assimilation

PDAF Parallel Data Assimilation Framework

Provide support for ensemble simulations

Augment model with data assimilation functionality

Provide methods for ensemble & variational data assimilation

Support easy integration of observation operators

PDAF Parallel Data Assimilation Framework

Open-source:
pdaf.awi.de
github.com/PDAF

Separation of concerns: Easy user uptake of new methods

Run from laptops to supercomputers

Apply data assimilation in real applications

Use to study assimilation algorithms

Teach data assimilation

Effect of DA on Ecosystem Indicators

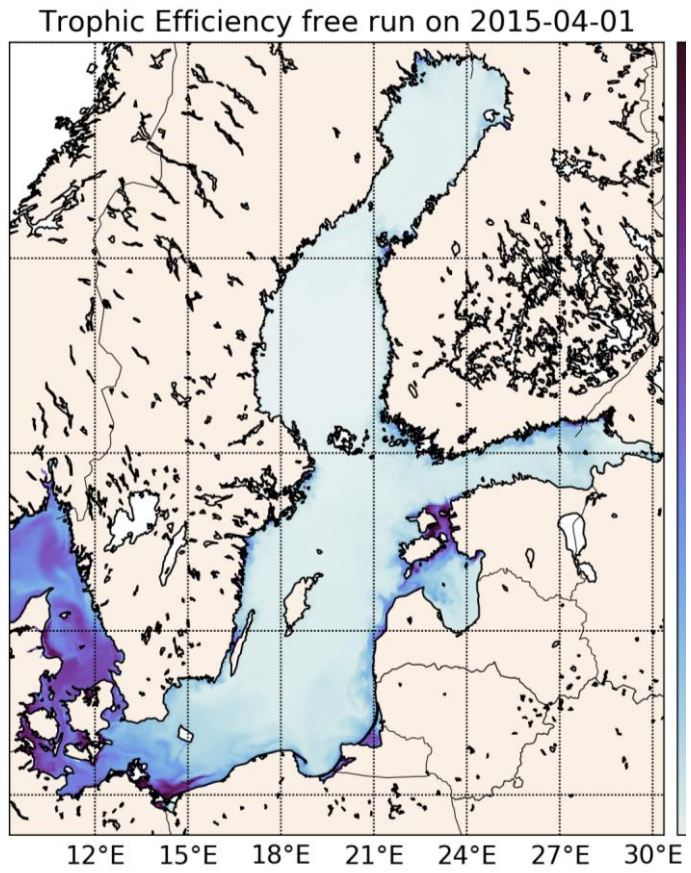
Trophic efficiency: zooplankton / phytoplankton

On April 1 only significant zooplankton in the transition zone to North Sea

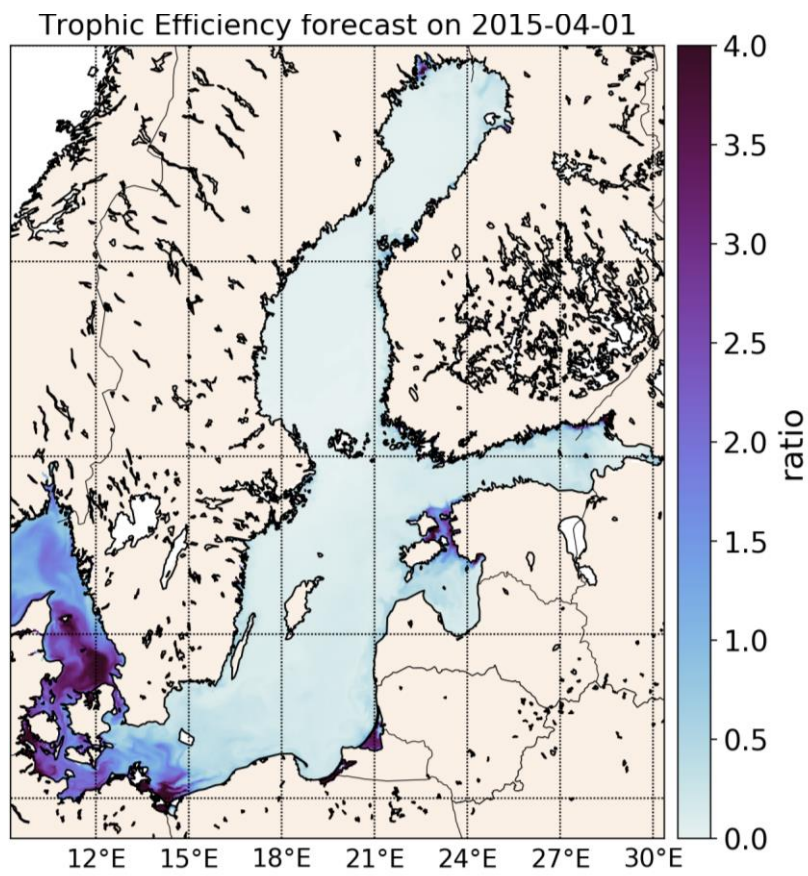
DA increases the ratio

Higher values further north e.g. in May

Free run on April 1



24h forecast on April 1

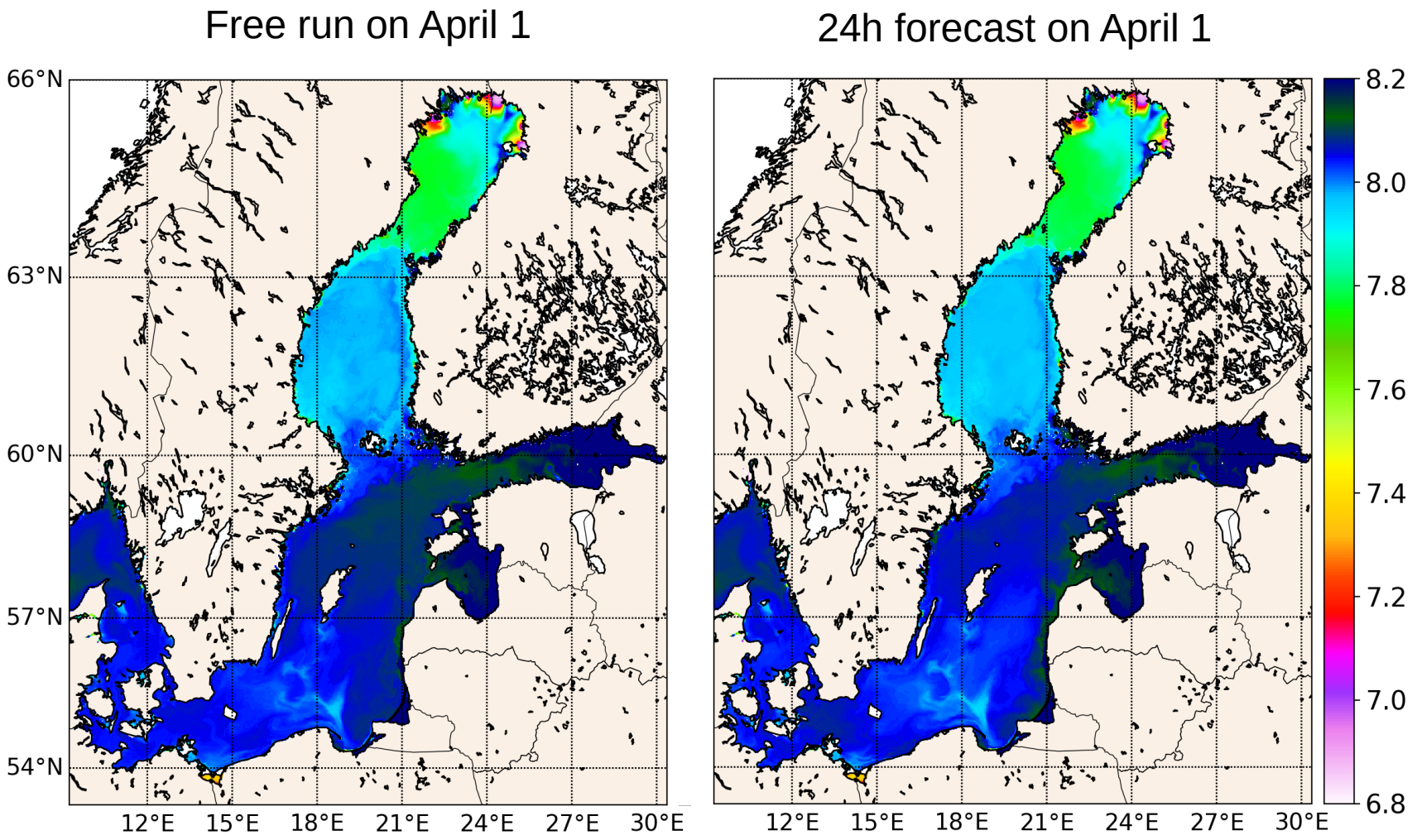


Effect of DA on Ecosystem Indicators

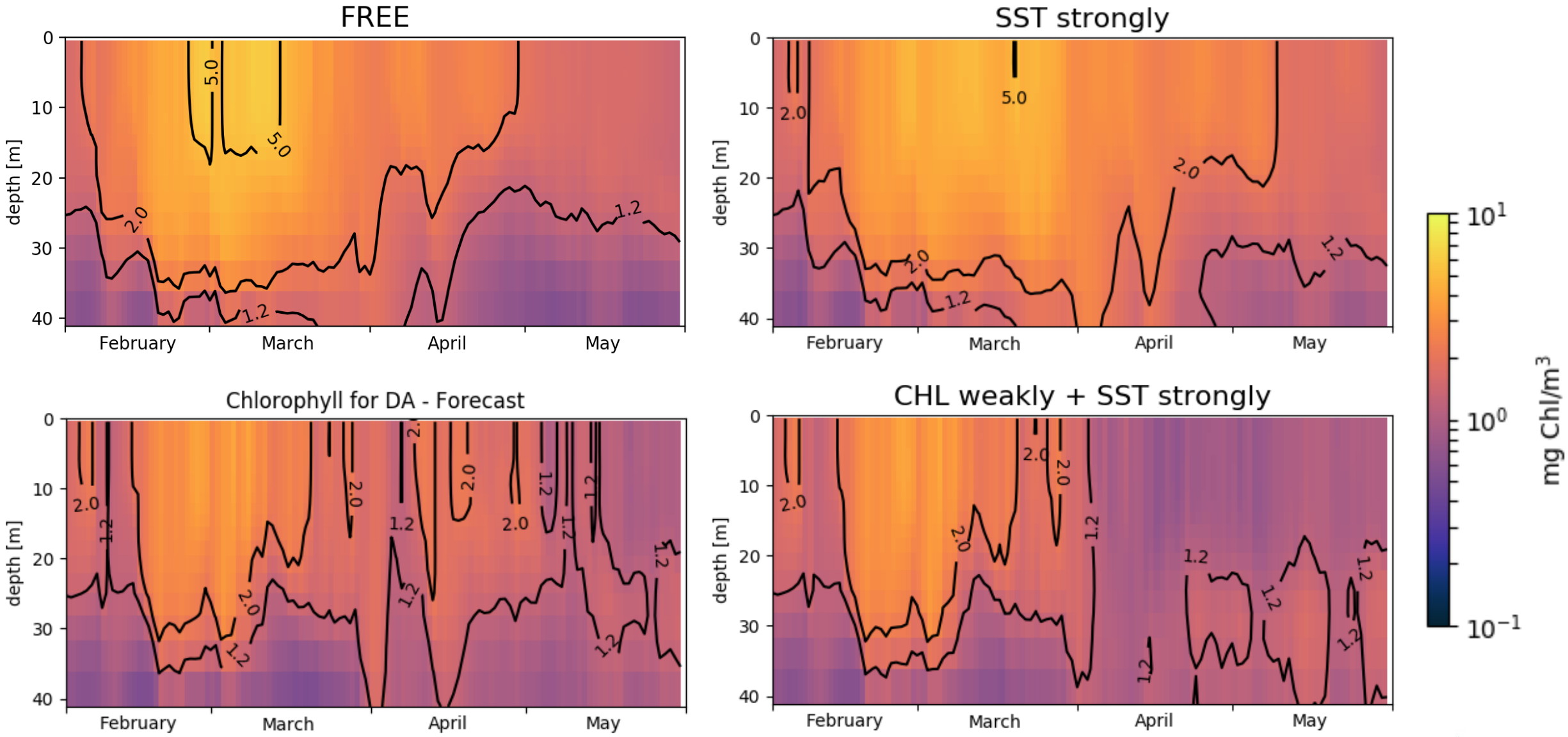
pH

Significant variations in the Baltic Sea.

The DA lowers pH slightly in the Baltic proper and Bothnian Sea

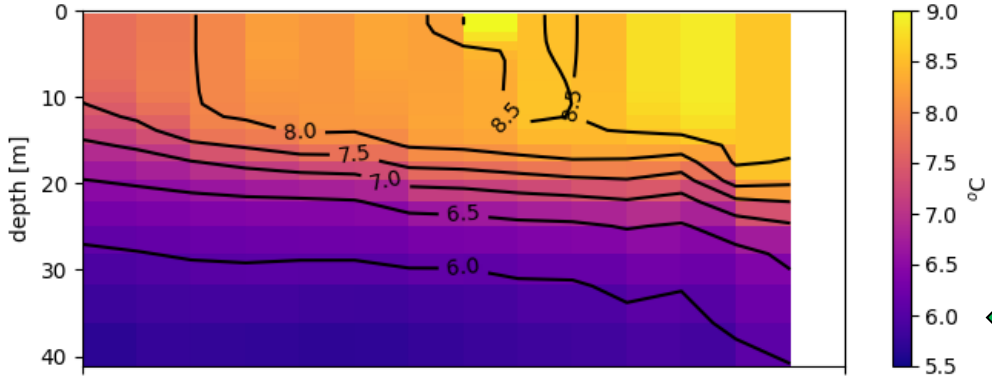


Effects on CHL Profiles at Station Arkona (southern Baltic)



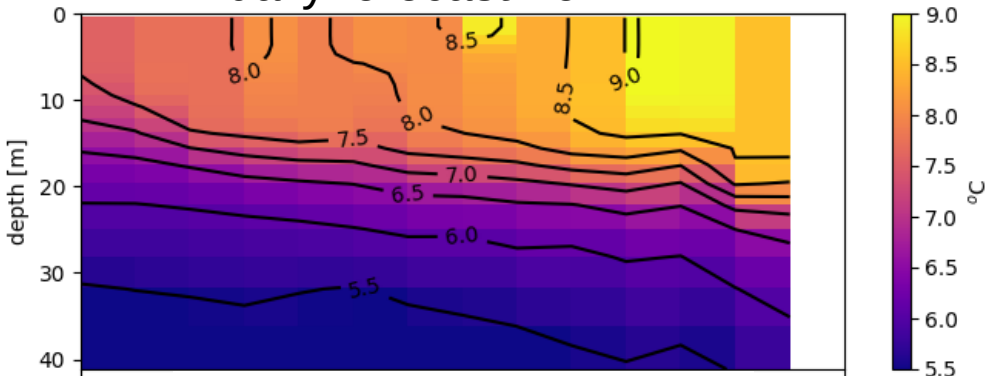
Profiles at station Arkona Basin – May 1 - 14

Free run

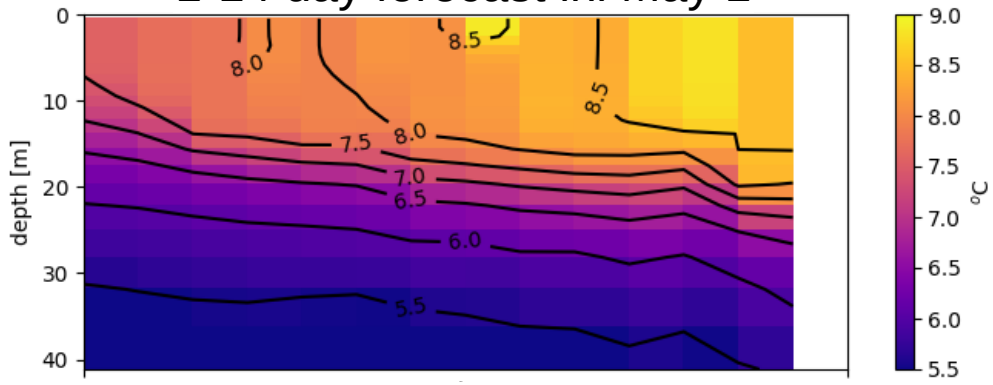


Temperature

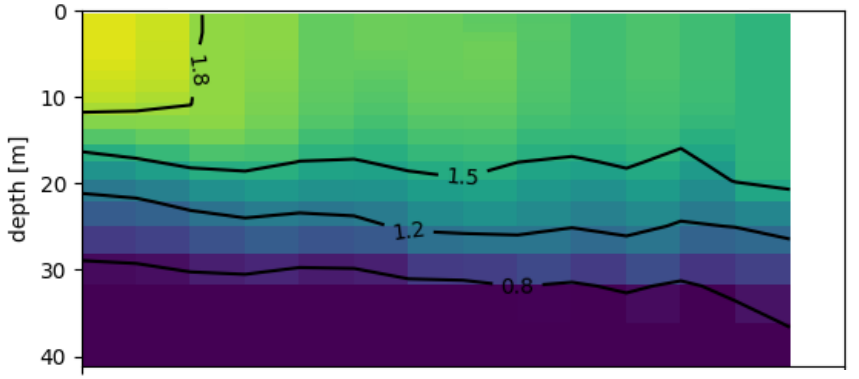
daily forecast from DA



1-14 day forecast ini May 1

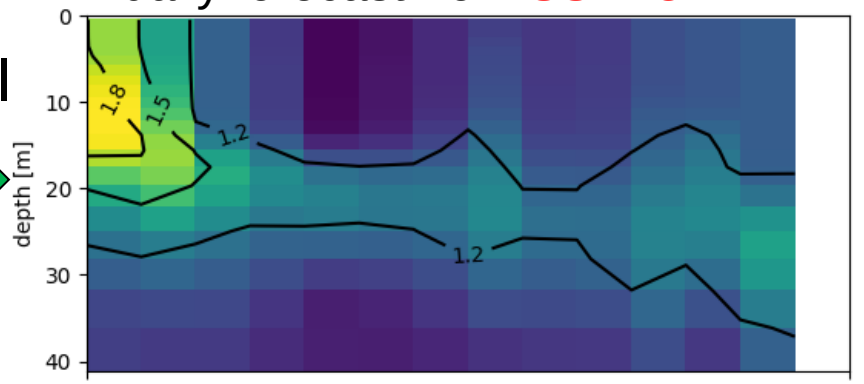


Free run

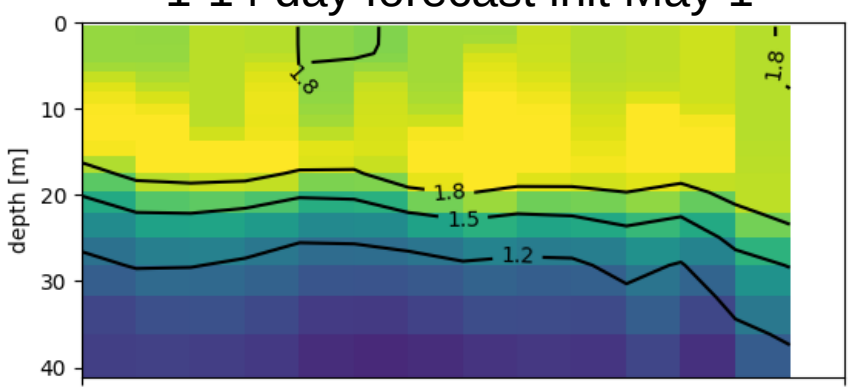


Chlorophyll

daily forecast from SST+CHL DA



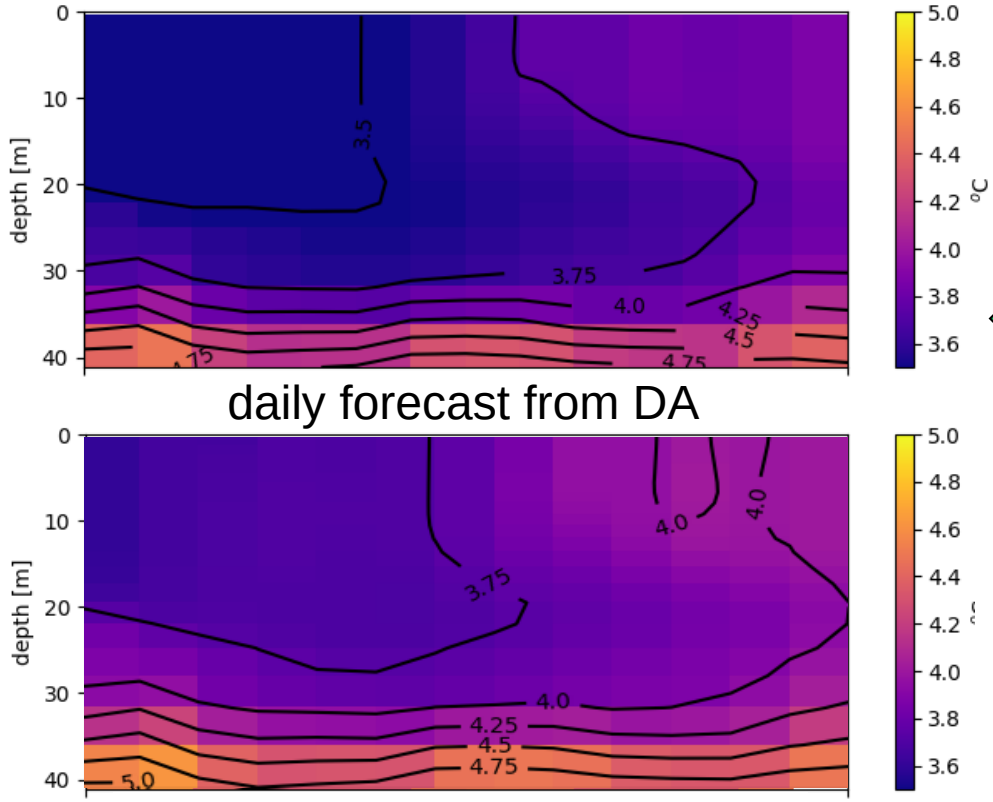
1-14 day forecast init May 1



en – Coupled physics-BC

Profiles at station Arkona Basin – March 1 - 14

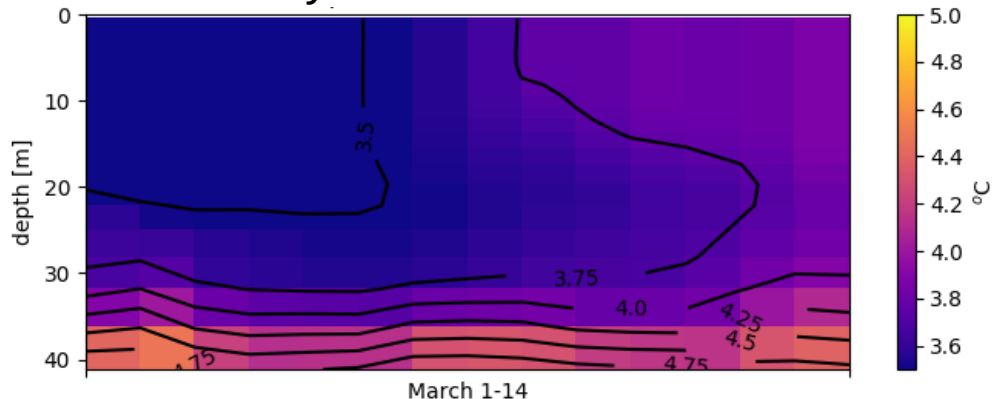
Free run



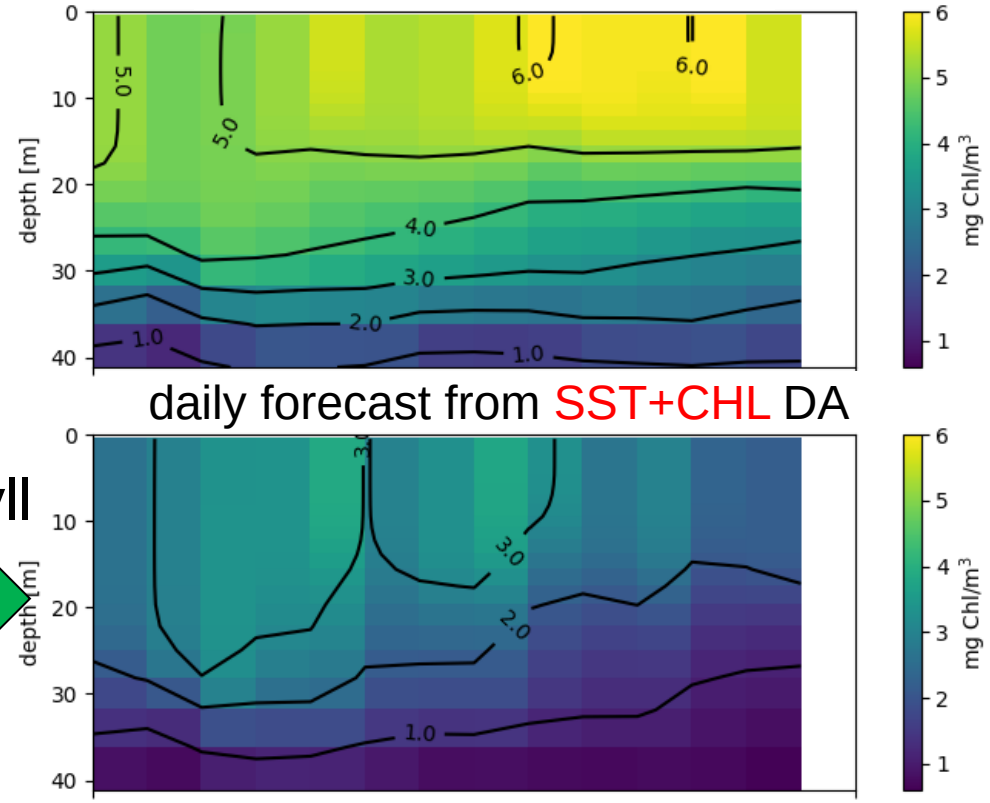
Temperature

daily forecast from DA

1-14 day forecast init. March 1



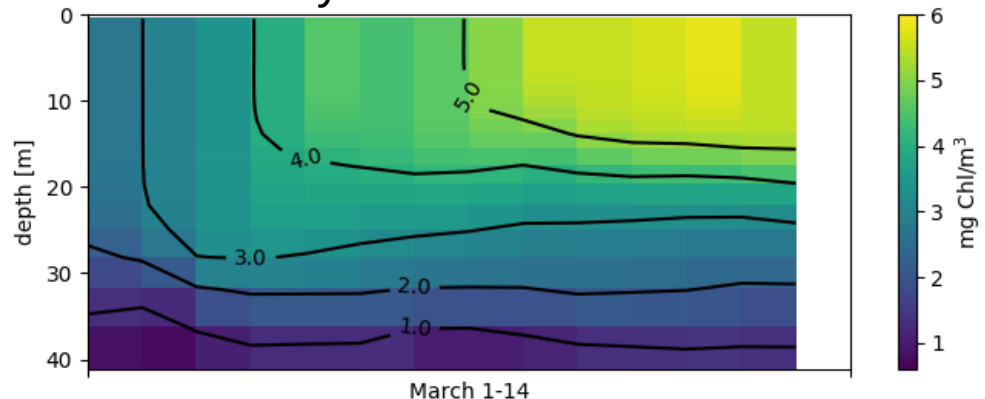
Free run



Chlorophyll

daily forecast from SST+CHL DA

1-14 day forecast init. March 1



en – Coupled physics-B