# **Ocean data assimilation and analysis**

DA training course 2024

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# Outline

- Ocean system and ocean observations
- NEMOVAR ocean data assimilation system
- Bias correction in ODA
- Assimilation of Sea-Level data
- Assimilation of SST data
- Assimilation of Sea-Ice data
- Ocean (re)analysis system and its applications



## Why do we need Ocean DA?

- Forecasting: initialization of coupled forecasts
  - NWP, monthly, seasonal, decadal
  - Calibration and reforecasts
- Verification/evaluation/co-design of Global Ocean observing network (OSE/OSSE)
- Climate applications
  - reconstruct & monitor the ocean (ECV/EOV);
  - study EEI and energy/water cycle;
- Towards coupled DA system (weakly -> quasi-strong -> strong ...)
- Other Commercial applications (oil rigs, ship route ...), safety and rescue, environmental (algii blooms, spills)

## **C**ECMWF

## Ocean for coupled forecasts



## Ocean versus Atmosphere

<u>Spatial/time scales</u> The radius of deformation in the ocean is small (~30km) compared to the atmosphere (~3000km). Time scales varies from hours (mixing) to decades (overturning circulations).

Ocean is a data sparse system, in-situ observation is limited and mostly covers upper ocean only, satellite observation only covers ocean surface and is only available for a relatively short period.

The ocean is forced at the surface and land boundary, by the wind/waves, heating/cooling and fresh-water fluxes

Uncertainty in forcing fluxes contributes to uncertainty in model results.

The ocean is strongly stratified in the vertical, especially near the surface. Although deep convection also occurs

Density is determined by Temperature and Salinity

The ocean has continental boundaries; dealing with them is not trivial in data assimilation

#### <mark>68</mark>/03/2024

## Ocean time scales: from hours to centuries



## Ocean spatial scales

The radius of deformation in the ocean is small (~30km) compared to the atmosphere (~3000km).

Satellite image of SST in the North Atlantic Ocean (from NOAA)



1/50 degree Ocean surface relative vorticity (CHASSIGNET and Xu, 2017)



mesoscale and submesoscale eddies

Ocean variables with various spatial scales: from hundred meters to hundreds of km

## Ocean is forced by external forcings

The ocean is forced at the surface and land boundary, by the wind/waves, heating/cooling and fresh-water fluxes. Uncertainty in forcing fluxes contributes to uncertainty in model results.



SST difference is mostly due to changes in ERA5 shortwave/longwave radiations. SSS difference is directly related with precipitation changes in ERA5

## Ocean is a data sparse system

in-situ observation is limited and mostly covers upper ocean only, satellite observation only covers ocean surface and is only available for a relatively short period.



## Ocean in-situ observations

New observations types are emerging: ALAMO, gliders, Deep Argo, BioArgo, drifter, saildrone ...





Argo operational cycle. [Argo 2018]

#### Moored buoys



Mammals!



[MEOP et al. 2015]

#### Ship based observations





## Satellite sea surface observations

- Satellite provide important observations on monitoring sea surface states (SST, SSS, sea-ice states, sea surface height, surface currents, ocean color, etc).
- These sea surface observations are essential input for ocean and seaice reanalysis system and works as complemental data sources to the ocean in-situ observing networks.
- Challenge to deal with various data densities among different in-situ types, and between in-situ and satellite observations.

## Sea-ice concentration



## Sea-ice thickness



# <text>

## Sea-Level Anomaly (Altimeter)





## Observations impact on the ocean state estimation



Assimilation of ocean in-situ observations helps to constrain the 3D ocean, therefore providing better estimation of the ocean initial condition for the coupled forecasting system

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## Ocean DA at ECMWF: NEMOVAR

#### NEMOVAR (CERFACS/ECMWF/INRIA/Met Office)

- En Variational DA system for **NEMO** ocean model.
  - Solves a linearized version of the full non-linear cost function.
  - Incremental **3D-Var FGAT** running operational, 4D-Var in research model
- Background correlation model based diffusion operators
- Background errors are correlated between different variables through **balance operator**

#### 3DVar-FGAT as in Daget et al 2009



Figure 1: Schematic illustration of the procedure used to cycle 3D-Var. On each cycle c, the model is integrated from  $t_0$  to  $t_N$  starting from a background initial condition  $\mathbf{x}_c^b(t_0)$  (grey dots) to produce the background trajectory  $\mathbf{x}_c^b(t_i)$  (black solid curve). The difference between the observations  $\mathbf{y}_{c,i}^o$  (black dots) and their background counterpart ( $\mathbf{H}_{c,i}\mathbf{x}_c^b(t_i)$ ) is computed (represented by the vertical thin dotted lines) for use in the 3D-Var FGAT minimization. After minimization, the model integration is repeated from the same initial condition  $(\mathbf{x}_c^b(t_0))$  but with the analysis increment applied using IAU. This produces the analysis trajectory  $\mathbf{x}_c^a(t_i)$  (grey dashed curve). The updated model state  $\mathbf{x}_c^a(t_N)$  at the end of cycle c is then used as the background initial condition for the next cycle c + 1 (grey dots).

Weaver et al 2003,2005; Balmaseda et al 2013; Daget et al 2009; Chrust et al., 2021 Mogensen et al 2012;



# NEMOVAR: Linearized Cost function

$$J[\delta \mathbf{w}] = \frac{1}{2} \delta \mathbf{w}^{\mathrm{T}} \mathbf{B}^{-1} \delta \mathbf{w} + \frac{1}{2} (\mathbf{G} \delta \mathbf{w} - \mathbf{d})^{\mathrm{T}} \mathbf{R}^{-1} (\mathbf{G} \delta \mathbf{w} - \mathbf{d})$$

 $y^{o} = \{(y_{0}^{o})^{T} \cdots (y_{i}^{o})^{T} \cdots (y_{N}^{o})^{T}\}^{T} \longrightarrow 4D \text{ observation array}$  $\delta w = w - w^{b} \longrightarrow w \text{ is the control vector}$  $d = y^{o} - G(w^{b}) \longrightarrow Departure vector$ 

 $G(\mathbf{w}) = \begin{pmatrix} \vdots \\ G_i(\mathbf{w}) \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ H_i[M(t_i, t_0)\{K(\mathbf{w})\}] \\ \vdots \end{pmatrix}$ 

- Balance operator: convert to w space, B becomes block diagonal, representing the spatial covariance model.
- Diffusion operator: The spatial covariances is specified by diffusion operator (Weaver and Courtier 2001)

Weaver et al 2003,2005 Daget et al 2009 Mogensen et al 2012 Balmaseda et al 2013



Solution:
$\delta \mathbf{w}^a \approx \mathbf{B} \mathbf{G}^T \left( \mathbf{G} \mathbf{B} \mathbf{G}^T + \mathbf{R} \right)^{-1} \mathbf{d}.$
$\delta \mathbf{x}^{a} = K \left( \mathbf{w}^{b} + \delta \mathbf{w}^{a} \right) - K \left( \mathbf{w}^{b} \right) \approx K \delta \mathbf{w}^{a}$
$\mathbf{x}^{\mathbf{a}}(t_i) = M(t_i, t_{i-1}) \big[ \mathbf{x}^{\mathbf{a}}(t_{i-1}), F_i  \delta \mathbf{x}^{\mathbf{a}} \big]$

IAU,Bloom et al 1996

## NEMOVAR: Linearized Balance Operator

Define the balance operator symbolically by the sequence of equations

Temperature 
$$\delta T = \delta T$$
  
Salinity  $\delta S = K_{S,T}^{b} \delta T + \delta S_{U} = \delta S_{B} + \delta S_{U}$   
SSH  $\delta \eta = K_{\eta,\rho} \delta \rho + \delta \eta_{U} = \delta \eta_{B} + \delta \eta_{U}$   
u-velocity  $\delta u = K_{u,p} \delta p + \delta u_{U} = \delta u_{B} + \delta u_{U}$   
v-velocity  $\delta v = K_{v,p} \delta p + \delta v_{U} = \delta v_{B} + \delta v_{U}$ 

Treated as approximately mutually independent without cross correlations

Density

Pressure

$$\begin{cases} \delta \rho &= \mathrm{K}_{\rho,T}^{\mathrm{b}} \, \delta T \,\, + \,\, \mathrm{K}_{\rho,S}^{\mathrm{b}} \, \delta S \\ \delta p &= \mathrm{K}_{p,\rho} \, \delta \rho \,\, + \,\, \mathrm{K}_{p,\eta} \, \delta \eta \end{cases} \} .$$

Weaver et al., 2005, QJRMS

## NEMOVAR: balance operator

Salinity balance (approx. T-S conservation To preserve the water mass properties following Troccoli and Haines (1999))

T<sub>an</sub>

T<sub>obs</sub>





T/S/SSH balance: vertical displacement of the profile.

## NEMOVAR: Background-Error covariances

**General B formulation in NEMOVAR** 

$$\mathbf{B} = \beta_m^2 (\mathbf{B}_{m_1} + \mathbf{B}_{m_2} + ...) + \beta_e^2 \mathbf{B}_e + \beta_E^2 \mathbf{B}_{EOF}$$
  
$$\mathbf{B}_{m_i} = \mathbf{K}_b \mathbf{D}_i^{1/2} \mathbf{C}_{m_i} \mathbf{D}_i^{1/2} \mathbf{K}_b^{\mathrm{T}}$$

- $B_m$  is modelled covariance matrix (can use multiple model to represent different scales)
- $B_e$  is a localized ensemble-based covariance matrix
- $B_{EOF}$  is a EOF-based covariance matrix
- $C_m$  is correlation matrix (including diffusion operator)
- $D_m$  is a diagonal matrix of variances (block-diagonal).



#### Horizontal correlation length-scales used in ORAP5

diffusion operator use diffusion tensor  $\kappa_m$  to represent a particular decorrelation length-scales

 $\mathbf{C}_X^{1/2} = \mathbf{\Gamma}_X^{1/2} \mathbf{L}_X^{1/2}$ 

## Ensemble Var DA with Hybrid-B

Generate an ensemble of analyses from an ensemble of background states and perturbed observations



- Ensemble DA perturbations simulate errors for the deterministic system;
- 3D-Var analysis for both deterministic and ensemble system;
- Observation and surface forcing perturbations as in ORAS5 (Zuo et al. 2017);
- Implementation of stochastic physics in NEMO (A. Storto, CMRE).

## **C**ECMWF

## BGE variances ( $\sigma^2$ ) in hybrid B

A hybrid background error variances  $\sigma^2$  in  $D_m$  contains modelled variances  $\sigma_m^2$  (parameterized  $\sigma_p^2$  + climatology  $\sigma_c^2$ ) and "error-of-the-day" estimated from ensemble spreads ( $\sigma_e^2$ )

Only climatological ensemble + error of the day 0.2 0.6 0.8 1.0 1.2 1.4 0.0 0.4 0.2 0 0.4 0.6 0.8 1.2 1.4 (°C)

EDA temperature spreads

Chrust et al., 2021

Ocean temperature spread at the surface from an Ensemble of Ocean Data Assimilations. The highest background errors are in western boundary current and Antarctic Circumpolar Current regions. This shows more details than without errors of the day, including a more detailed structure of sub-mesoscale eddies with much sharper fronts, and a hint of tropical instability waves in the tropical Pacific Ocean

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## Bias correction in ODA

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## Why do we need bias correction in ODA

To mitigate changes in the observing system. E.g. salt content drift in the Southern Ocean during pre-Argo period due to lack of in-situ observations.



## Why do we need bias correction in ODA

To correct systematic errors in models/forcing/boundary conditions, and biases introduced by DA system. E.g. add BC can greatly reduced SST biases, especially in the Gulf Stream regions where the 1/4 degree NEMO model has persistent bias.



#### SST biases (February) in the Gulf Stream Extensions

## **Bias Correction scheme**

Bias term include two parts, (a) a-priori bias  $(\overline{b}_i)$  for systematic errors, and (b) a temporal evolution bias term  $(b'_c)$  for slow evolving signals (Balmaseda et al, 2007)



$$\overline{b}_i = \overline{b}_{i-1} + \overline{\delta x_i^a}$$

A-priori bias term can be estimated with iterative approach, where  $\overline{b}_0 = 0$ , and  $\overline{\delta x_i^a}$  is averaged increments from the i<sub>th</sub> iteration, which should approach to zero with i increases

Slow varying term, estimated online from assimilation increments

$$b_c' = \alpha b_{c-1}' - A\delta x_{c-1}^a$$

A is a Linear transformation matrix from the state vector increment  $(\delta x_c^a)$ to bias control vector;  $\alpha$  is the memory factor

The bias correction is used to modify the tendencies of the nonlinear model used in the background and analysis outer loops, so the time evolution of the background and analysis states can be expressed as

$$\mathbf{x}_{c}^{b}(t_{i}) = M(t_{i}, t_{i-1}) [\mathbf{x}_{c}^{b}(t_{i-1}), \mathbf{b}_{c-1}],$$
  
$$\mathbf{x}_{c}^{a}(t_{i}) = M(t_{i}, t_{i-1}) [\mathbf{x}_{c}^{a}(t_{i-1}), \mathbf{b}_{c-1}, F_{i} \delta \widetilde{\mathbf{x}}_{c}^{a}]$$

## A-priori bias term for different systems

A-priori biases ( $\overline{b}_1$ ) in (left) ORAS5 and (right) ORAP6



Among other differences, ORAS5 uses ERA-int forcing while ERA5 forcing is used in ORAP6

Vertical profile of  $\bar{b}_T$  in ORAS5 and ORAP6 in the North Atlantic Ocean



## **Temporal variable bias term**

The latitude dependent partition coefficients determine the proportion of online bias corrections applied directly on T/S, and on pressure term. These values ensure that at low latitude the dominant bias term is pressure correction.



Figure 3: Latitude-dependent linear reduction coefficients as applied on online bias correction terms in equations 6 and 7: blue line -  $d^{tr,T/S}$ , reduction coefficients that apply to direct temperature and salinity corrections (different for ORAS4 and ORAP5); and green line -  $a^{p,T/S}$ , reduction coefficients that apply to pressure bias correction.

## Impact of bias correction on ocean reanalysis



*Temperature RMSE: 0-1000m* 

Bias correction in ODA is essential, and in particular important for mitigating spurious signals introduced due to changes in the observing system

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# **Assimilation of Sea Surface Height (SSH)**





Altimeter measures SSH (respect reference ellipsoide) Model represents **n** (ssh referred to the

Geoid)

## SSH-Geoid= η

Geoid was poorly known (until recent years)

Alternative: Assimilate Sea Level Anomalies (SLA) respect a time mean

Obs: SSH anomalies = SSH-MSSH = Obs SLA Mod: η anomalies =  $\eta - MDT$  = Mod SLA

```
Where: MSSH= Temporal Mean SSH ;
MDT = Temporal Mean of model SL Mean
Dynamic Topography
MSSH – Geoid = MDT
```

# **Assimilation of SSH: MDT**

- $MDT_m$  : model MDT as mean( $SSH_m$ ), mean model biases not corrected (Balmaseda et al., 2013)
- *MDT<sub>o</sub>*: observation MDT as mean(*SSH<sub>o</sub>*), observation bias not corrected (Waters et al., 2015 and Lellouche et al., 2018)
- *bias corr*. *MDT*<sub>o</sub> : observation biases corrected (Lea et al., 2008)

 $MDT_m - MDT_o$  (in m)





# **Assimilation of SSH: pre-processing**

- The SLA along track data has very high spatial (9-14km) resolution for the operational ocean assimilation systems.
  - Features in the data which the model can not represent
  - "Overfitting" to SLA obs
- This can be dealt with in different ways:
  - Inflate the observation error
  - Construction of "superobs" or thinning



## Thinning of SLA obs



# **Assimilation of SSH: impact on ocean states**

Assimilation of SSH improves simulated ocean states

- Global mean sea-level changes •
- Regional sea-level changes •
- Subsurface temperature and salinity ٠
- Large-scale ocean circulations •

**Т ΔRMSE (О-В)**:



#### Temporal correlation (monthly) to AVISO data **ORAS5** assim. SSH – not assim. SSH **ORAS5-NoAlti** Zuo et al., 2018 cci2 - gcb8 sossheig : Correl (1993-2014) cci2 - gc73 sossheig : Correl (1993-2014) 60N 60W 100E 160W 60W 100E 160W Longitude (m): Min= -1.00, Max= 1.00, Int= 0.02 Longitude (m): Min= -1.00, Max= 1.00, Int= 0.02 $0.40 \quad 0.44 \quad 0.48 \quad 0.52 \quad 0.56 \quad 0.60 \quad 0.64 \quad 0.68 \quad 0.72 \quad 0.76 \quad 0.80 \quad 0.84 \quad 0.88 \quad 0.92 \quad 0.96 \quad 1.00 \quad 0.96 \quad$

0.40 0.44 0.48 0.52 0.56 0.60 0.64 0.68 0.72 0.76 0.80 0.84 0.88 0.92 0.96 1.00

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# **Assimilation of SST: nudging**

A simple nudging scheme to L4 objective analysis data (e.g. OSTIA)



# Impact of SST nudging

- Overall very effective except for some areas with weak vertical stratification
- Not accounting complicated error characteristics in the L4 SST analysis
- Not accounting vertical correlation when apply SST constrain in the surface





#### SST bias: free run - OSTIA



# Assimilation of L4 SST with NEMOVAR

- Assimilation of L4 SST (OSTIA) with Ens. 3DVar and hybrid-B approach
- SST DA leads to reduced SST biases on the Gulf Stream extensions w.r.t nudging method
- Hybrid-B with a MLD dependent vertical tensor is essential in SST DA



## Biases in SST



## SST DA (hybrid-B)



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## Sea-ice DA with single-category LIM2 model

Sea-Ice Concentration data from L4 analysis is assimilated through 3DVar scheme in the OCEAN5 system

- Treated as univariate
- Pre-thinned via regular or stratified random sampling
- Assimilated through outer-loop coupling in NEMO-LIM2





## Sea-ice DA with multi-category SI3 model



Figure 1.1.: Representation of the ice pack, using multiple categories with specific ice concentration  $(a_l, l = 1, 2, ..., L)$ , thickness  $(h_l^i)$ , snow depth  $(h_l^s)$ , vertical temperature and salinity profiles  $(T_{kl}^i, S_{kl}^s)$  and a single ice velocity vector (u).

Considerations with SIC DA in SI3 (multi-category sea-ice model with melt ponds)

- How to distribute increments among different thickness categories
- Where to apply sea-ice increments in the ice time-stepping scheme
- Introduce thermodynamic balance between sea-ice and ocean state variables
- Grow sea-ice from open water with DA increment
- Interaction between sea-ice increment and ice advection



#### **ORAS6** prototype daily sea-ice concentration

fixed thickness, iiti 5.0 20100605 siconc Ice fraction min 0.0 max 0.996999979019165





## Assimilation of L3 sea-ice data



L4 analysis: with filtering, masking, infilling to produce a gap-free product

with 10km resolution there is ~1 milion obs per day from L3 OSI-SAF, with no infilling created observation

#### soicecov soicecov 120°W 120°W Assimilation of SIC data in SIC bias (1980-2016) "" 90°W Ref data: OSI-SAF 430 60°W 60°W 30°W 30°W 30°E 30°E In percent -0.17 -0.13 -0.09 -0.05 -0.01 0.03 0.07 0.11 0.15 0.19 -0.17 -0.13 -0.09 -0.05 -0.01 0.03 0.07 0.11 0.15 0.19 iicethic iicethic 120°W 120°W SIT bias (2011-2016) Ref data: CS2SMOS<sup>9</sup> 90°W merged data 60°W 60°W z 30°W 30°W 30°E 30°E In m -1.9 -1.5 -1.1 -0.7 -0.3 0.1 0.5 0.9 1.3 1.7 -1.5 -1.1 -0.7 -0.3 0.1 0.5 0.9 1.3 1.7 -1.9

Positive impact on sea-ice states Without SIC DA

#### With SIC DA

ORAS5 leads to improved sea-ice state performance in both sea-ice concentration and sea-ice thickness

## Nudging sea-ice thickness (SIT)

$$SIT^{n} = SIT^{m} - \left[\frac{\Delta t}{\tau}\left(SIT^{m} - SIT^{o}\right)\right]$$

where  $SIT^n$  is the nudged thickness,  $SIT^m$  is the modelled thickness,  $SIT^o$  is the observed thickness, tau is the nudging coefficient

Difference in forecast Integrated Ice Edge Error (2011-2016, verified against OSI-401b)

## with SIT nudging – No SIT nudging

Difference in Integrated Ice Edge Error



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## **ECMWF Ocean Reanalysis-analysis system**



OCEAN5 is the 5<sup>th</sup> generation of ECMWF ocean and sea-ice ensemble reanalysis-analysis system (Zuo et al., 2018, 2019).

- Ocean: NEMOv3.4
- Sea-ice: LIM2
  - Resolution: <sup>1</sup>/<sub>4</sub> degree with 75 levels
  - Assimilation: 3DVAR-FGAT
  - 5 ensemble member
  - Forcing: ERA-int

## **Application of Ocean analysis: coupled forecasts**

OCEAN5 provides ocean and sea-ice initial conditions for all ECMWF coupled forecasting system: (ENS, HRES, Seasonal). OCEAN5 also provides SST and SIC conditions for the ECMWF atmospheric analysis system (Browne et al., 2018)



- Gain about 2 months in ENSO prediction
- Without Ocean observation and DA, we would lose about 15 years of progress.

## Applications: observing system co-design and impact studies

Remove CTD/XBT/MBT

180

120°W

## Maps of normalized RMSD of Temperature (upper 700m) in OSEs

60°N

30°5

60°S

#### Remove Moored buoys a)



#### Remove Argo c)

#### 60°E 120°F Remove all in-situ d)



0.05 0.25 0.45 0.65 0.85 1.05 1.25 1.45 1.65 1.85

Zuo et al., 2019, Ocean Science

RMSD w.r.t a reference reanalysis, in which all in-situ data are assimilated.

During 2009/2010, there was a transient 30% weakening of the AMOC driven by anomalies in geostrophic and Ekman transports (Roberts et al., 2023)

#### Maximum AMOC fluxes (in Sv) at 26.5 N





## Applications: monitoring climate signals

ORAs provides continuous coverage of the global oceans constrained by law of physics and observations input, and therefore can resolve higher frequency variability in ocean than methods that rely primarily on in situ data.



ORAS4 suggests that there is more heat absorbed by the deeper ocean after 2004.

## ORAS5 NRT monitoring of OHC300



Longitude-time, 1-yr daily record

https://charts.ecmwf.int/catalogue/packages/oras5\_nrt/

ECMWF

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# Summary

- Data assimilation in the ocean serves a variety of purposes, from climate monitoring to initialization of coupled model forecasts and ocean mesoscale prediction.
- This lecture dealt mainly with ocean DA for **initialization of coupled forecasts and reanalyses**, with a global ocean model in climate resolution and use **NEMOVAR** as an example.
- Compared to the atmosphere, **ocean observations are sparse**. The main source of information are temperature and salinity profiles, sea level and ocean wave from altimeter, SST/SIC/SIT from satellite and in-situ.
- ECMWF NEMOVAR uses a incremental **3DVar-FGAT** configuration and linearized cost function. The BGE covariance is modelled use **balance** operator and **diffusion** operator.
- Data assimilation changes **the ocean mean state**. consistent ocean reanalysis requires an explicit treatment of model biases.
- Assimilation of ocean observations reduces the large uncertainty due to model and forcing errors. It improves the initialization of coupled forecasts in NWP, and provides calibration and initialization for reforecast for seasonal forecasts and decadal forecasts.

## **Further Readings**

## **Ocean Data assimilation**

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