









Ocean data assimilation



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This DA lecture mostly deals with physical oceanography and the ocean circulation, but does not address:

- ocean wave forecasting
- tidal/storm surge forecasting
- ocean chemistry and water quality
- Fish, whales, sharks, jellyfish...

The slides are designed to be more or less "self-sufficient" ==> wordy sometimes, not extremely fluent

























"Observation-centered" approach



Outline Texte du titre

- 1. Atmospheric vs oceanic data assimilation
 - 1.1. History and culture
 - 1.2. Observations
 - 1.3. Dynamics and models
- 2. "Model-centered" data assimilation
 - 2.1. Operational oceanography
 - 2.2. Ocean models
 - 2.3. Observations of the ocean
 - 2.4. Ensemble Kalman filter implementations
- 3. "Observation-centered" data assimilation
 - 3.1. Assimilation of images
 - 3.2. Altimetric products and the SWOT mission
 - 3.3. Mapping balanced motions with a nudging technique
 - 3.4. Eddy/wave separation with a 4DVar technique



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Meteorology:



Meteorology:

 strong and historical rooting in forecasting issues Oceanography:

 Forecasting is an issue, but not the only one (importance of observation-centered DA)



Meteorology:

- strong and historical rooting in forecasting issues
- the most advanced field for high-dim. DA

- Forecasting is an issue, but not the only one (importance of observation-centered DA)
- less maturity than in meteorology



Meteorology:

- strong and historical rooting in forecasting issues
- the most advanced field for high-dim. DA
- Dedicated manpower

- Forecasting is an issue, but not the only one (importance of observation-centered DA)
- less maturity than in meteorology
- much less manpower



Meteorology:

- strong and historical rooting in forecasting issues
- the most advanced field for high-dim. DA
- Dedicated manpower
- DA is culturally accepted

- Forecasting is an issue, but not the only one (importance of observationcentered DA)
- less maturity than in meteorology
- much less manpower
- DA is always questioned



If a user needs a time series of global maps of Sea Level pressure, what will her choice be?



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An ECMWF reanalysis, probably.



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An ECMWF reanalysis, probably.

If a user needs a time series of global maps of SSH, what will her choice be?

DUACS products are the most widely used by oceanographers. Until 2024, they were made from nadir altimeter data with a space-time linear interpolation.



Meteorology:



Meteorology:

 Large number of observations Oceanography:

 Comparatively small number of observations



Meteorology:

- Large number of observations
- Satellite observations are 3D

- Comparatively small number of observations
- Satellite observations are 2D



Meteorology:

- Large number of observations
- Satellite observations are 3D
- Very often, observation operators are complex

- Comparatively small number of observations
- Satellite observations are 2D
- Very often, observation operators are simple



Atmospheric vs oceanic data assimilation Dynamics and models



Atmospheric vs oceanic data assimilation Dynamics and models

Phenomenon	Length scale L	Velocity scale U	Time scale T	
Atmosphere:				
Sea breeze Mountain waves Weather patterns Prevailing winds Climatic variations	5–50 km 10–100 km 100–5000 km Global Global	1-10 m/s 1-20 m/s 1-50 m/s 5-50 m/s 1-50 m/s	12 h Days Days to weeks Seasons to years Decades and beyond	
Ocean: Internal waves Coastal upwelling Large eddies, fronts Major currents Large-scale gyres	1–20 km 1–10 km 10–200 km 50–500 km Basin scale	0.05-0.5 m/s 0.1-1 m/s 0.1-1 m/s 0.5-2 m/s 0.01-0.1 m/s	Minutes to hours Several days Days to weeks Weeks to seasons Decades and beyond	



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Atmospheric vs oceanic data assimilation Dynamics and models

The scales particularly relevant for weather predictions and important for climate require more/finer observations in the ocean.

	Length scale	Velocity scale	Time scale
Phenomenon	Length scale	U	Т
Atmosphere:			
Sea breeze	5–50 km	1–10 m/s	12 h
Mountain waves	10-100 km	1–20 m/s	Days
Weather patterns	100-5000 km	1–50 m/s	Days to weeks
Prevailing winds	Global	5–50 m/s	Seasons to years
Climatic variations	Global	1–50 m/s	Decades and beyond
Ocean:			
Internal waves	1–20 km	0.05-0.5 m/s	Minutes to hours
Coastal upwelling	1–10 km	0.1 - 1 m/s	Several days
Large eddies, fronts	10-200 km	0.1 - 1 m/s	Days to weeks
Major currents	50-500 km	0.5–2 m/s	Weeks to seasons
Large-scale gyres	Basin scale	0.01–0.1 m/s	Decades and beyond



Atmospheric vs oceanic data assimilation Dynamics and models

* The scale of eddies is set by the Rossby radius of deformation:

 $L_{\rho} = \frac{NH}{2\Omega}$

- N: Brunt-Vaïsala frequency
- H: layer thickness
- Ω : Earth rotation
- * ~30 km in the ocean, ~1000 km in the atmosphere
- * Ocean weather simulations require high resolution models!



(Chelton et al, 1998)



Atmospheric vs oceanic data assimilation Dynamics and models



https://github.com/ocean-next/eNATL60



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Operational oceanography Use of data assimilation

Operational oceanography started about 25 years ago.





Operational oceanography Use of data assimilation

The main goal is real-time monitoring and prediction of the state of the ocean, including:

- Currents (shipping, sea operations, regattas...)
- Primary production (marine resources, fishing)
- Sea ice (shipping)
- Temperature (climate, weather forecasting...)

Like weather forecast centers, OO centers provide useful information to scientists: reanalyses, targeted forecasts for field campaigns, etc.



Operational oceanography Mercator Ocean International

Mercator Ocean International:

- The French center of OO;
- Created in 1995;
- Located in the area of Toulouse, about 50 agents;
- officially appointed by the European Commission on 11 November, 2014 to implement and operate the Copernicus Marine Service (CMEMS).
- Development in collab with research labs
- <u>http://www.mercator-ocean.fr/</u>



Operational oceanography Mercator Ocean International



À propos Services

Océanographie opérationnelle

Actualités & Agenda Ressources Presse

Q

Q

Marine heatwave forecasts – 8 February

Andreia Carvalho

Marine Heatwave Bulletin

The marine heatwave bulletin provides forecasts and analysis of marine heatwave events across the globe and throughout the year. Used datasets include observations (satellite sea surface temperature maps) and numerical model analyses (assimilating satellite and in situ observations) to derive marine heatwave forecasts for a 10-day period. [1] This week's forecasts were produced using as a comparison the marine heatwave situation on 28/01/2024.

• Forecasts for 8 February



Marine heatwave categories for 8 February 2025 (global ocean). GL012. Source: Mercator Ocean International



Category and geographical extent differences for 8 February 2025 (global ocean). GLO12. Source: Mercator Ocean International

Rechercher

Rechercher.

Catégories

Sélectionner une catégorie

Étiquettes

2D3D 7e continent climat CMEMS CMEMS workshop CNES CNRS Connaissance de l'environnement océanique Copernicus copernicus marine Copernicus Marine Service Croissance Bleue Decade Collaborative Centre Digital

Twin Ocean DTO EU Green week Global Ocean Week 2016 GOW LEGOS Livre marée noire Météo France NAOS Ocean Day Ocean Decade ocean governance Ocean prediction Ocean Science océan digital Partenariat Pierre Bahurel platique pollution Press 2015 RUTW satellite satellites Sea Plastics Sentinel Sentinel-3A Toulouse UN Ocean Decade Usine Nouvelle wakashio Workshop Copernicus



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Ocean models Primitive equations

Conservation of:

• momentum

- Mass
- Salt
- Temperature
- Equation of state

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = fv - \frac{1}{\rho} \frac{\partial p}{\partial x} + K_u \frac{\partial^2 u}{\partial z^2}$$
$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -fu - \frac{1}{\rho} \frac{\partial p}{\partial y} + K_v \frac{\partial^2 v}{\partial z^2}$$
$$-\frac{\partial p}{\partial z} = \rho g$$
Nonlinear terms

div $\overrightarrow{u} = 0$

$$\rho \frac{DS}{Dt} = \text{div} \ (K_{\text{s}} \text{grad } S)$$
$$\rho C_{\text{v}} \frac{DT}{Dt} = \text{div} \ (K_{\text{T}} \text{grad } T)$$
$$\rho = \rho(T, S, p)$$

+ auxiliary conditions



Ocean models Discretization

- Mercator operational model: NEMO 1/12°
- Number of gridpoints:

 $4322 \times 3059 \times 75 \sim 10^9$

 1 year of simulation costs 414 Gb memory, 90000 CPU hours, 1Tb storage (daily outputs)

3059 2295 2000 1530 766

OPERATIONNEL 1/12, PREVISION, velocity 92m

2162

3242

1081

1

1

4322


Ocean models Uncertainties: example of forcing conditions



Yellow: atmospheric

Grey: oceanic

Green: parameterizations

White: physical processes



Ocean models Uncertainties: example of forcing conditions



mm/day



Ocean models Uncertainties: example of forcing conditions



c

<figure><figure>

PRECIPITATION (mm/day) Climatological mean, map of difference CFSR - GPCP-v2.2 (1979-2010)



d

PRECIPITATION (mm/day) Climatological mean, map of difference NCEP-R2 - GPCP-v2.2 (1979-2010)







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Observations of the ocean In situ observation #1: profilers







Observations of the ocean In situ observation #1: profilers



ARGO = network of profiling floats

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Observations of the ocean In situ observation #1: profilers

- +++: Spatial coverage, vertical information, autonomy
- : needs maintenance, some regions hard to sample, poor sampling



http://www.argo.ucsd.edu/



Observations of the ocean In situ observation #2: Moorings

- +++ : time sampling, vertical information, autonomy
- - : expensive to build and maintain, poor spatial coverage





http://www.whoi.edu/virtual/oceansites/network/index.html 44



Observations of the ocean In situ observation #3: surface drifters

- +++ : Spatial coverage, autonomy
- - : needs maintenance, some regions hard to sample, poor sampling





A drifter measures surface temperature and currents. http://www.aoml.noaa.gov/ http://www.nefsc.noaa.gov/



Observations of the ocean In situ observation #4: marine mammals

- +++: access to poorly observed area, vertical information
- - : limited spatial and temporal coverage

A miniaturized CTD (Conductivity-Temperature-Depth) probe





observed areas!





https://www.aviso.altimetry.fr/en/home.html 47



analysed height anomaly difference : VAR SLAANA on 08-01-2003



Orbit of Jason: Cycle of 10 days.



Orbit-1 (Jason)

H=1336km i= 66°

(sub-)cycles (days) : 0.9 3.3 9.9



Orbit of Envisat and Saral:

Cycle of 35 days



Orbit-3 (Envisat, Saral H=782km i=98°

(sub-)cycles (days) : 1.0 3.0 17.5 35.0







Observations of the ocean Satellite observation #2: SST

- IR radiometer (e.g. AVHRR)
- Microwave radiometer (e.g. AMSR-E)

- Both at 1-km resolution.
- MW insensitive to clouds but less sensitive and easy to calibrate.

Some IR sensors are on-board geostationary satellites (res. 5 km). Most are polar orbiting.







Two issues with satellite SST from the DA viewpoint:

- Cloud detection
- SST is a "skin" temperature (representation error)



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EnkF implementations Kalman filter equations

Initialization: \mathbf{x}_0^f and \mathbf{P}_0^f **Analysis step:**

$$\begin{split} \mathbf{K}_{k} &= (\mathbf{H}_{k}\mathbf{P}_{k}^{f})^{T}[\mathbf{H}_{k}(\mathbf{H}_{k}\mathbf{P}_{k}^{f})^{T}+\mathbf{R}_{k}]^{-1}, \\ \mathbf{x}_{k}^{a} &= \mathbf{x}_{k}^{f}+\mathbf{K}_{k}(\mathbf{y}_{k}^{o}-\mathbf{H}_{k}\mathbf{x}_{k}^{f}), \\ \mathbf{P}_{k}^{a} &= (\mathbf{I}-\mathbf{K}_{k}\mathbf{H}_{k})\mathbf{P}_{k}^{f}. \end{split}$$

Forecast step:

$$\mathbf{x}_{k+1}^f = \mathbf{M}_{k,k+1} \mathbf{x}_k^a, \\ \mathbf{P}_{k+1}^f = \mathbf{M}_{k,k+1} \mathbf{P}_k^a \mathbf{M}_{k,k+1}^T + \mathbf{Q}_k.$$



EnkF implementations Kalman filter equations





* In the forecast step, each member is advanced with the numerical model:

$$\mathbf{x}_{k+1,i}^f = M_{k,k+1}(\mathbf{x}_{k,i}^a) + \eta_{k,i}$$



EnKF analysis step

- At the analysis step, each member is corrected using observations.
- Different analysis schemes exist:
 - stochastic/deterministic,
 - algebra in observation/ensemble space,
 - Serial/batch processing of observations,
 - With/without adaptive scheme at some point,
 - etc



EnkF implementations Flavors of EnKF: illustration



Deliverable 3.1

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SANGOMA European project, http://www.data-assimilation.net/) 58



EnkF implementations Flavors of EnKF: illustration



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EnkF implementations Flavors of EnKF: A simple view

- OI methods
 - Forecast of 1 (mean) state
 - Analysis using statistics from a fixed ensemble
- Stochastic EnKF
 - Correction of each state with perturbed observations
- Deterministic EnKFs
 - Correction of mean and anomalies without perturbing observations



EnkF implementations Flavors of EnKF: A simple view

- Ocean DA: O(10⁶ 10⁸) variables, O(10³ 10⁵) obs.
- Ensemble Kalman filters used in operational oceanic DA systems:
 - Ensemble OI (Mercator-Océan, France; Bureau of Meteorology, Australia; and others)
 - Deterministic EnKF (NERSC, Norway)



Ensemble Optimal Interpolation

- Ensemble OI:
 - Only a mean state is propagated with the model;
 - The error modes (ensemble anomalies) are the same at all analysis steps.
- - - : no estimation of uncertainties;
- +++: computationally affordable, robust (no collapse), more "physically-based" than historical OI with analytical covariance functions.



- Localization aims at delimiting in space the impact of an observation;
- Localization is necessary for several reasons:
 - To avoid long-range corrections due to spurious long-range correlations, themselves due to the small size of the ensemble;
 - To artificially increase the rank of the covariance matrix and provide more degrees of freedom to the corrections;
 - To make computation possible in some cases.



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EnKF implementations Localization



(Brankart et al, 2011) 65



EnKF implementations Incremental Analysis Updating (IAU)

Model not involved during analysis: discontinuity, balance problems and shocks at restart possible.

Right: spurious wave generated by the assimilation of a single observation.





- An empirical solution is Incremental Analysis Updating (IAU, Bloom et al, 1996)
- IAU consists in computing corrections at the analysis step, then re-running the ensemble over the forecast window, adding incrementally to each member its correction under the form of a forcing term.

Here, IAU is run from the middle of the previous forecast window to the middle of the next forecast window.

Continuity is guaranteed (perhaps at the expense of quality of the analysis).





EnkF implementations Incremental Analysis Updating (IAU)

Figure: spatially averaged zonal velocity U in the Gulf Stream zone.

Black: free run

Red: EnOI

Green: EnOI with IAU



FIG. 12. Same as in Fig. 11, but at a 55-m depth (model depth level 5) from Julian day 15678 (4 Dec 1992) to 16038 (5 Dec 1993): black line represents FREE run, red line represents INT run, and green line represents IAU run.



Some quantities must be conserved. Example: mass.

div $\mathbf{u} = 0$

- Bogus: a fictitious observation of div **u**, equal to 0.
- Bogus can be used in regions where the assimilation makes things worse...



EnKF implementations Gaussian anamorphosis

 Sometimes the distribution of some variables does not follow a Gaussian law;



Distribution of silicate at 3 different dates (over a large oceanic domain)

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- Sometimes the distribution of some variables does not follow a Gaussian law;
- But the EnKFs work better with Gaussian variables;
- Gaussian anamorphosis: transformation of a distribution into a Gaussian distribution.



EnKF implementations Gaussian anamorphosis

- The transformation can be analytical or empirical;
- On the opposite figure, the transformation is empirical;
- Such transformation can be performed on each variable individually.




- After transformation, the EnKF analysis is performed;
- Then, the physical variables are retrieved by the inverse transformation.



EnKF implementations Gaussian anamorphosis



Obs. update at BATS station (65°W-32°N) using a perfect PHY observation. Prior ensemble (red), mean (green square), linear regression line (thin green line), truth (big blue dot), posterior ensemble (blue dots). Left: EnKF analysis; Middle: analysis in the transformed state space; Right: Anamorphosis-EnKF posterior. The thick green line on the right is the transformation of the thin green line on the middle.



EnkF implementations About the observation error covariance matrix

$$\mathbf{P}^f = \mathbf{S}^f \mathbf{S}^{f^T}$$

 The EnKF correction is either calculated with (using a serial processing of observations)

$$\delta \mathbf{x} = \mathbf{S}^{f} (\mathbf{H} \mathbf{S}^{f})^{T} \left[(\mathbf{H} \mathbf{S}^{f}) (\mathbf{H} \mathbf{S}^{f})^{T} + \mathbf{R} \right]^{-1} (\mathbf{y} - \mathbf{H} \mathbf{x}^{f}),$$

• Or, with $\Gamma = (\mathbf{HS}^{f})^{T} \mathbf{R}^{-1} (\mathbf{HS}^{f})$

$$\delta \mathbf{x} = \mathbf{S}^{f} \left[\mathbf{I} + \mathbf{\Gamma} \right]^{-1} (\mathbf{H}\mathbf{S}^{f})^{T} \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}\mathbf{x}^{f}).$$



- For simplification, all ocean DA systems consider the observation error covariance matrix diagonal.
- To minimize the impact of the neglected correlations, it is common to inflate the variances (in the Norwegian operational system, they are multiplied by 2 for the update of the anomalies).
- On the other hand, many efforts are dedicated to the construction of the state error covariance matrix.



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Assimilation of images Optical images





Ocean color sensors detect chlorophyll.

A phytoplankton bloom captured near Alaska by Operational Land Imager (OLI) on Landsat 8 (NASA).

AVHRR composite image of SST.



Assimilation of images Optical images



AVHRR composite image of SST.

Example: Optic flow methods

$$\frac{\partial T}{\partial t} + \nabla T \cdot \mathbf{w} = 0$$

with T observed and w driven by a shallow-water model:

$$\left(\begin{array}{ccc} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= fv - g' \frac{\partial h}{\partial x} \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} &= -fu - g' \frac{\partial h}{\partial y} \\ \frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (vh)}{\partial y} &= 0 \end{array} \right)$$



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Altimetric products and the SWOT mission Sea Level anomaly maps

Present-day nadir altimetry is processed to provide gridded maps of Sea Level Anomaly. This is done with the DUACS algorithm at CNES/CLS, implementing statistical interpolation.

These maps resolve scales of 200 km and 10 days.





https://www.aviso.altimetry.fr/en/home.html 81



Altimetric products and the SWOT mission The SWOT mission

- SWOT: Surface Water and Ocean Topography
- Satellite mission launched in 2022
- Revolutionary altimetric observation: 120 km-wide swath
- Pixel of 2 km, revisit 10 days (mismatch)



KNC Swath KNC KNC Swath 5 - 15 km Alt. 5 - 15 km



Altimetric products and the SWOT mission The SWOT mission



Le Gulf Stream vu par Copernicus et le satellite SWOT



Altimetric products and the SWOT mission The SWOT mission

- Mismatch between spatial and temporal coverage of SWOT
- Expectation that dynamics must be considered in the interpolation
- ==> data assimilation



decorrelation time as a function of wavelength



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Mapping balanced motions with a nudging technique Methodology

- Method: Back-and-forth nudging (BFN) with a 1.5-layer quasi-geostrophic (QG) model.
 - Why a simple 1.5-layer QG model?

It is a simple model able to capture a large part of mesoscale ocean dynamics as observed by altimetry.

• Why BFN?

It is a conceptually simple method.

The QG dynamics is governed by a single variable, almost directly observed.

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Mapping balanced motions with a nudging technique Methodology

(QG) Forward propagation:	$\frac{\partial X}{\partial t} = M(X,t) \qquad X(0) = x_0$	
Forward nudging:	$\frac{\partial X}{\partial t} = M(X,t) + K(y^{obs} - X)$	
(QG) Backward propagation:	$\frac{\partial X}{\partial t} = M(X,t) \qquad X(T) = x_T$	
Backward nudging:	$\frac{\partial X}{\partial t} = M(X,t) - K(y^{obs} - X)$	

BFN algorithm (Auroux et al., 2008): combination of the **forward nudging** and the **backward nudging** in an **iterative** process over a temporal window



Mapping balanced motions with a nudging technique

Experimental setup



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Mapping balanced motions with a nudging technique Experimental setup



 4 conventional along-track altimeters (Nadirs)

SWOT

- No errors considered



Mapping balanced motions with a nudging technique Results

Example with SWOT + Nadirs constellation



2013-05-01



Nudging nadir altimetry only

Results

SSH on 20230410





Nudging is so flexible

Results





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Problem statement

	Phenomenon	Length scale L	Velocity scale U	Time scale T
	Atmosphere:			
	Sea breeze Mountain waves Weather patterns Prevailing winds Climatic variations	5–50 km 10–100 km 100–5000 km Global Global	1-10 m/s 1-20 m/s 1-50 m/s 5-50 m/s 1-50 m/s	12 h Days Days to weeks Seasons to years Decades and beyond
	Ocean:			
SWOT Conventional nadir altimetry	Internal waves Coastal upwelling Large eddies, fronts Major currents Large-scale gyres	1–20 km 1–10 km 10–200 km 50–500 km Basin scale	0.05-0.5 m/s 0.1-1 m/s 0.1-1 m/s 0.5-2 m/s 0.01-0.1 m/s	Minutes to hours Several days Days to weeks Weeks to seasons Decades and beyond



Problem statement and experimental setup

BM: Balanced motions IT: Internal tides

Reference

$$\eta_{truth} = \eta_{truth}^{BM} + \eta_{truth}^{IT}$$
$$\eta_{truth}^{BM}(t_0) = \frac{1}{2T} \int_{t_0-T}^{t_0+T} \eta_{truth}(t) dt$$
$$\eta_{truth}^{IT}(t_0) = \frac{1}{T} \int_{t_0-T}^{t_0+T} \eta_{truth}(t) \cdot \cos\left(\frac{2\pi}{T}t\right) dt$$

Observation One snapshot every 75 h (=3d+3h), free of noise



Simulation: Ponte et al, 2017



Method: coupled BM and IT estimations

BM estimation

- Dynamics
- 1.5-layer quasi-geostrophic model

$$\partial_t q + J(\psi, q) = 0$$

where:
$$\psi = \frac{g}{f}\eta$$
 , $q = \nabla^2 \psi - \frac{1}{{L_R}^2}\psi$

Data assimilation technique

BFN, based on **nudging** equation: $\partial_t q + J(\psi, q) - K(q_{obs} - q) = 0$

Le Guillou, F., Metref, S., Cosme, E., Ubelmann, C., Ballarotta, M., Le Sommer, J., & Verron, J. (2021). Mapping Altimetry in the Forthcoming SWOT Era by Back-and-Forth Nudging a One-Layer Quasigeostrophic Model, *Journal of Atmospheric and Oceanic Technology*, *38*(4), 697-710.

IT estimation

• Dynamics

1-layer linear shallow water model...

$$\partial_t u - fv = -g \partial_x \eta$$
$$\partial_t v + fu = -g \partial_y \eta$$
$$\partial_t \eta = -H_e(\partial_x u + \partial_y v)$$

- ...forced by open boundary conditions
- Data assimilation technique:

4Dvar, minimizing the cost function:

 $J(p) = ||\eta_{obs} - \eta||^2$ where *p* : model parameters (*H_e* and boundary conditions)



4DVar control parameters: illustration





Alternating minimization



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Results: convergence





- Convergence reached after 10 iterations.
- Throughout iterations, both components are progressively separated.
- IT estimation looks very similar to the truth

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Results: estimation of nonstationary IT

0.0 days



Le Guillou et al, 2021



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Problem statement