Ocean data assimilation

OACOS master's program
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Acknowledgements

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* These names hide many others who indirectly contributed, particularly from LGGE/MEOM, Mercator-Océan, LJK/MOISE, and NASA/JPL.
* And thank you for the invitation to give this talk.

Scope of this lecture

* This DA lecture mostly deals with:
  * the ocean circulation
  * the ocean primary production
* This lecture does not address:
  * ocean wave forecasting
  * tidal/storm surge forecasting
  * ocean chemistry and water quality
  * Fish, whales, sharks, jellyfish…

Scope of this lecture

* This lecture is biased towards operational applications:
  * Realistic models;
  * Real observations;
  * Practical implementation of DA;
  * And a very limited amount of theory.

Operational oceanography: the primary user of ocean data assimilation

* Operational oceanography started about 20 years ago;
* 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 turn to provide useful information to scientists: reanalyses, targeted forecasts for field campaigns, etc.

Mercator-Océan

* 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 set up the European ocean-monitoring service (pilot phase: MyOcean EU project, 2009-2015)

Mercator-Océan and research groups

* To develop its operational system, Mercator-Océan relies on the research community in the labs. In France, these are primarily (non-exhaustive list in almost arbitrary order):
  * LGGE/MEOM (Grenoble)
  * LOCEAN (Paris)
  * LPO (Brest)
  * LEGOS (Toulouse)
  * CERFACS (Toulouse)
  * Météo-France (Toulouse)
  * etc

Web sites

* Mercator-Océan: http://www.mercator-ocean.fr/
* MyOcean: http://www.myocean.eu/
* GODAE Oceanview: https://www.godae-oceanview.org/
* DRAKKAR project: http://www.drakkar-ocean.eu/
* GFDL Ocean modeling: http://ocean-modeling.org/
* Coriolis data center: http://www.coriolis.eu.org/

Textbooks

* Advanced data assimilation for Geosciences, Eds. E. Blayo, M. Bocquet & E. Cosme, Oxford, 2014
* Data assimilation, Making sense of observations, Eds W. Lahoz, B. Khattatov & R. Ménard, Springer, 2010
* Ocean Weather Forecasting, Eds. E. Chassignet & J. Verron, Springer, 2006

Outline

* Ocean models
* Observations of the ocean
* Ocean DA using Ensemble Kalman filters
* Ocean DA using variational methods
* Mercator-Océan operational DA system
* Future challenges

Ocean models

* Primitive equations
* Scales
* Horizontal discretization
* Vertical discretization
* Uncertainties
* Biogeochemistry

Primitive equations

Conservation of:

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

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

$$-\frac{\partial p}{\partial z} = \rho g$$

- momentum

$$\mathrm{div}\ \vec{u} = 0$$

- Mass

$$\rho\frac{DS}{Dt} = \mathrm{div}\ (K_{\mathrm{S}}\mathrm{grad}\ S)$$

- Salt

$$\rho C_{\mathrm{v}}\frac{DT}{Dt} = \mathrm{div}\ (K_{\mathrm{T}}\mathrm{grad}\ T)$$

- Temperature

$$\rho = \rho(T, S, p)$$

Equation of state

+ auxiliary conditions

Primitive equations

Conservation of:

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

- momentum

Nonlinear terms

$$\mathrm{div}\ \vec{u} = 0$$

- Mass

$$\rho\frac{DS}{Dt} = \mathrm{div}\ (K_{\mathrm{S}}\mathrm{grad}\ S)$$

- Salt

$$\rho C_{\mathrm{v}}\frac{DT}{Dt} = \mathrm{div}\ (K_{\mathrm{T}}\mathrm{grad}\ T)$$

- Temperature

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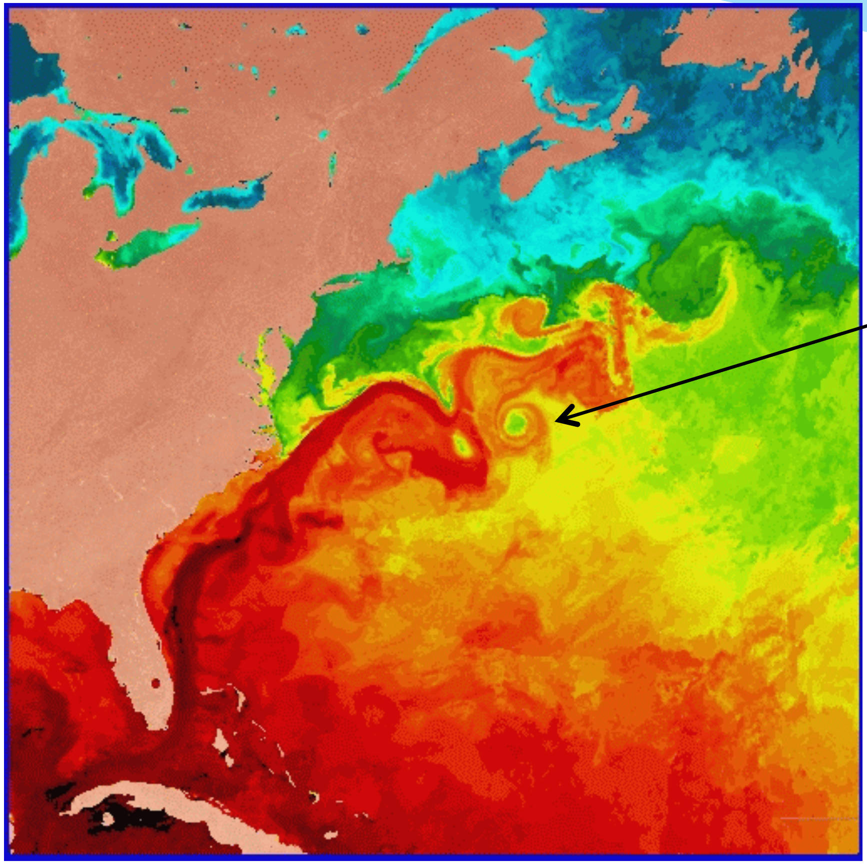
Equation of state

+ auxiliary conditions

Primitive equations



Due to nonlinear terms

Primitive equations

* Why does this matter for DA?
  * Most tractable DA methods are designed for linear or weakly nonlinear systems;
  * A wide range of scales co-exist in the dynamics;
  * Representing the circulation accurately requires high-resolution models.

Scales

Phenomenon	Length scale L	Velocity scale U	Time scale T
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

Scales

Scales particularly relevant for weather predictions and important for climate too.

Phenomenon	Length scale L	Velocity scale U	Time scale T
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Scales

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

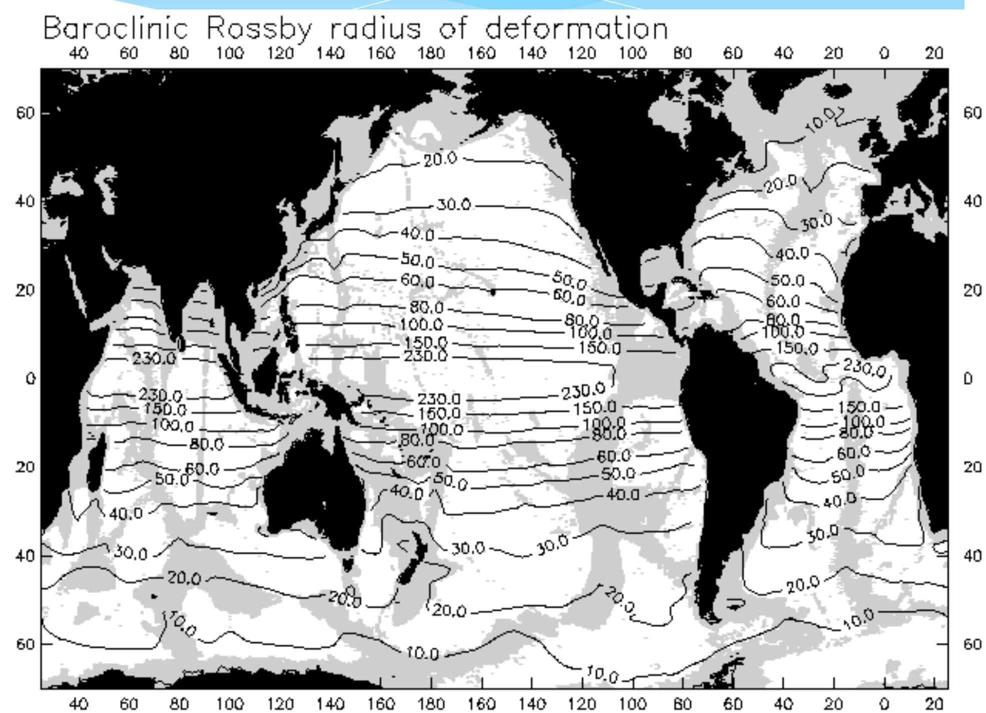
$$L_\rho = \frac{NH}{2\Omega}$$

N: Brunt-Vaïsala frequency

H: layer thickness

Ω: Earth rotation

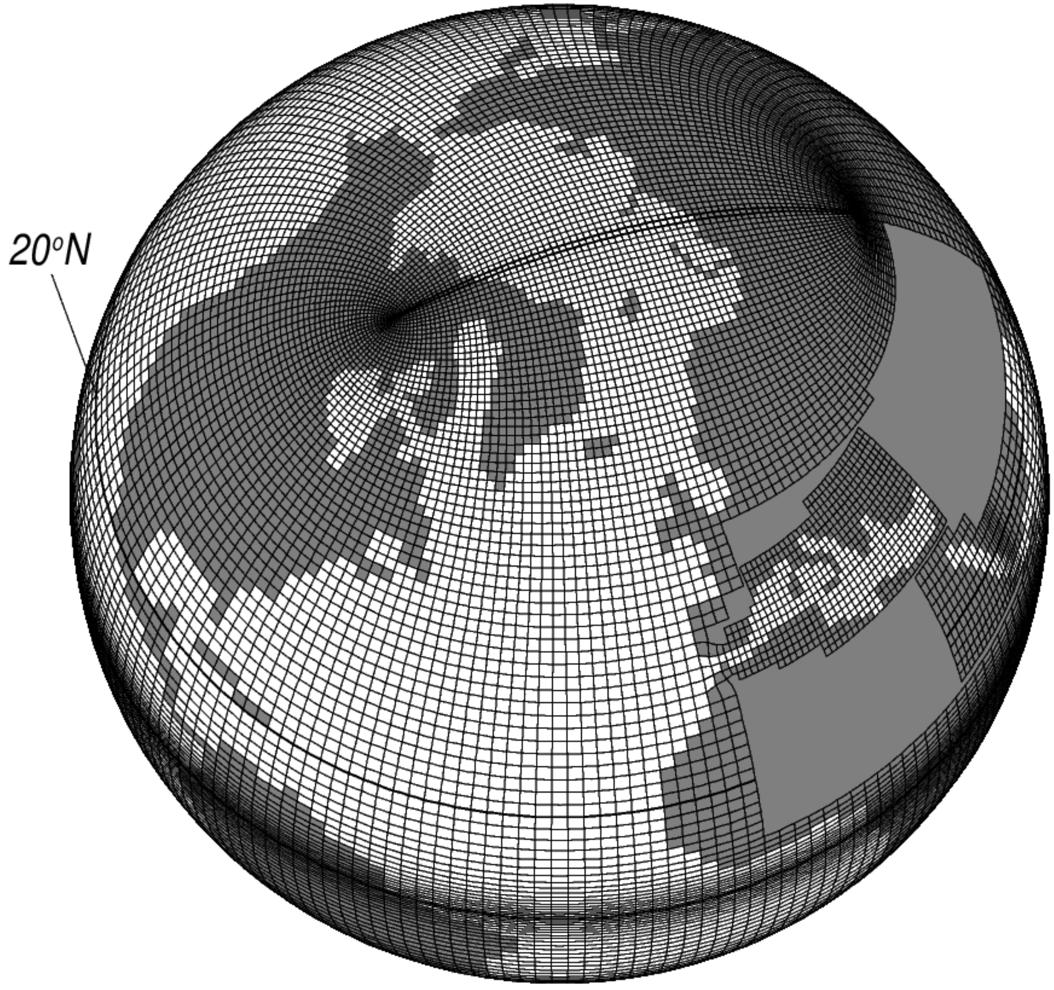
* ~30 km in the ocean, ~1000 km in the atmosphere
* Ocean weather simulations require high resolution models!



(Chelton et al, 1998)

Horizontal discretisation

- Figure: NEMO ORCA2 grid (2°)
- In 2015, operational version at 1/12° at Mercator-Océan
- Regional configuration at higher resolutions
- Resolution is pushed ahead…

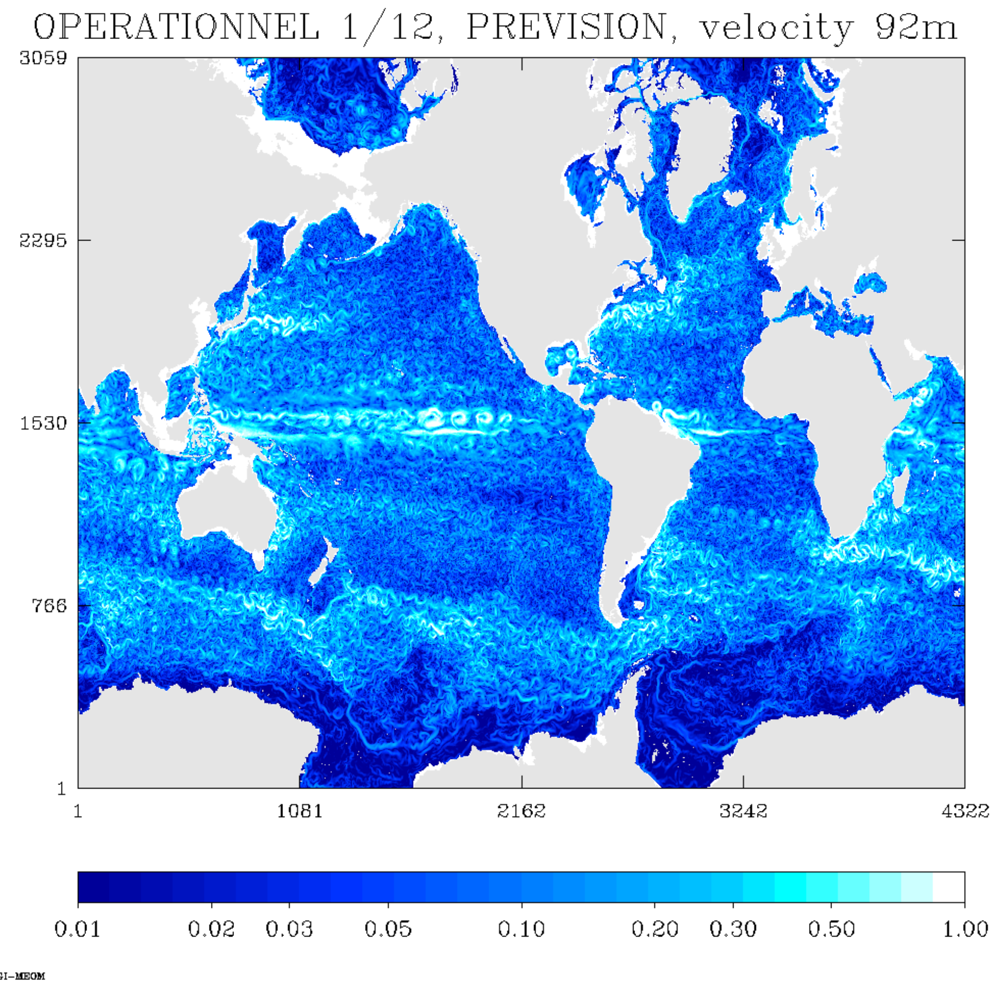


Horizontal discretisation

* 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)

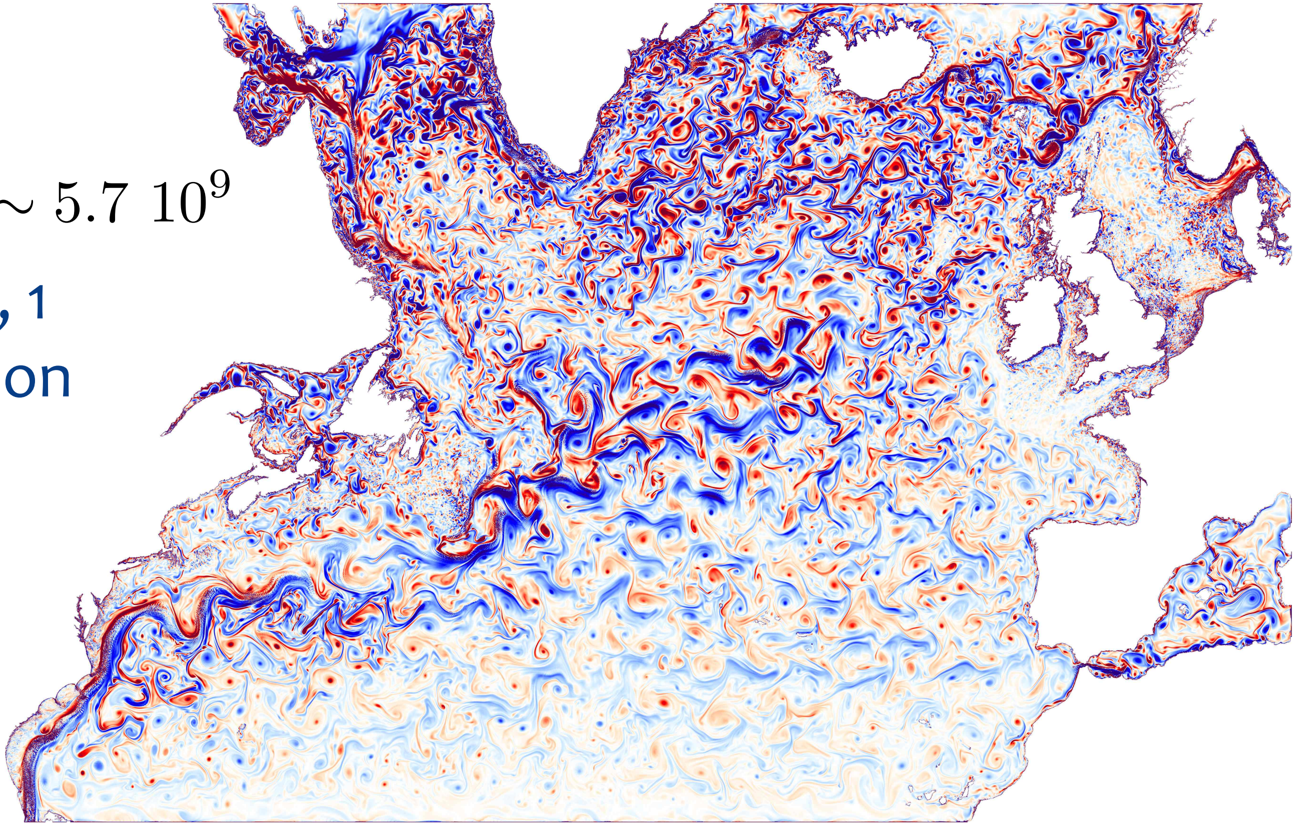


Horizontal discretisation

* NATL60
* Gridpoints:

$$5454 \times 3474 \times 300 \sim 5.7\ 10^9$$

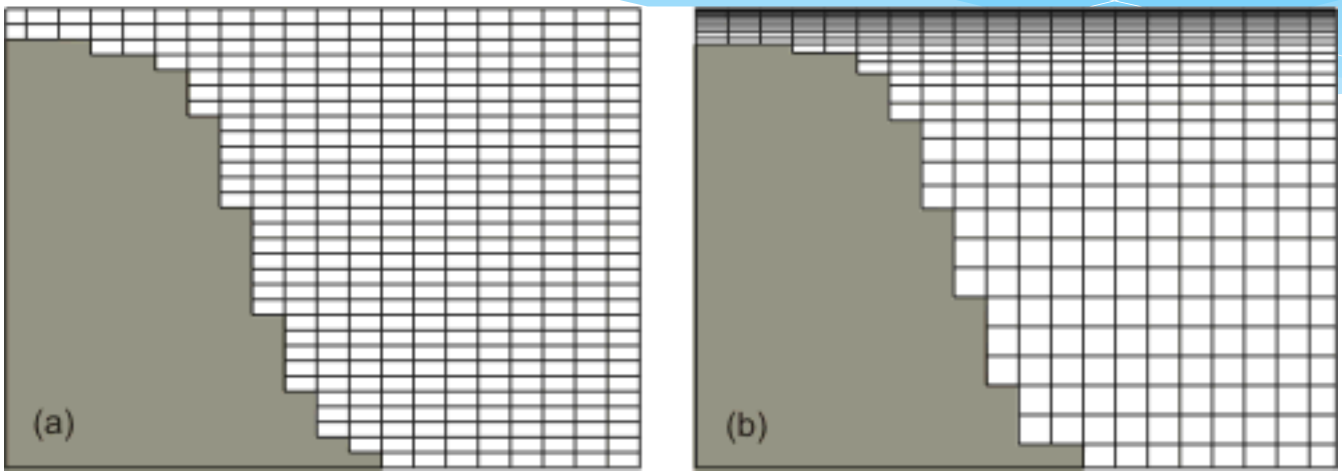
* 13000 processors, 1 month of simulation takes 1 day
* Full storage impossible



Horizontal discretisation

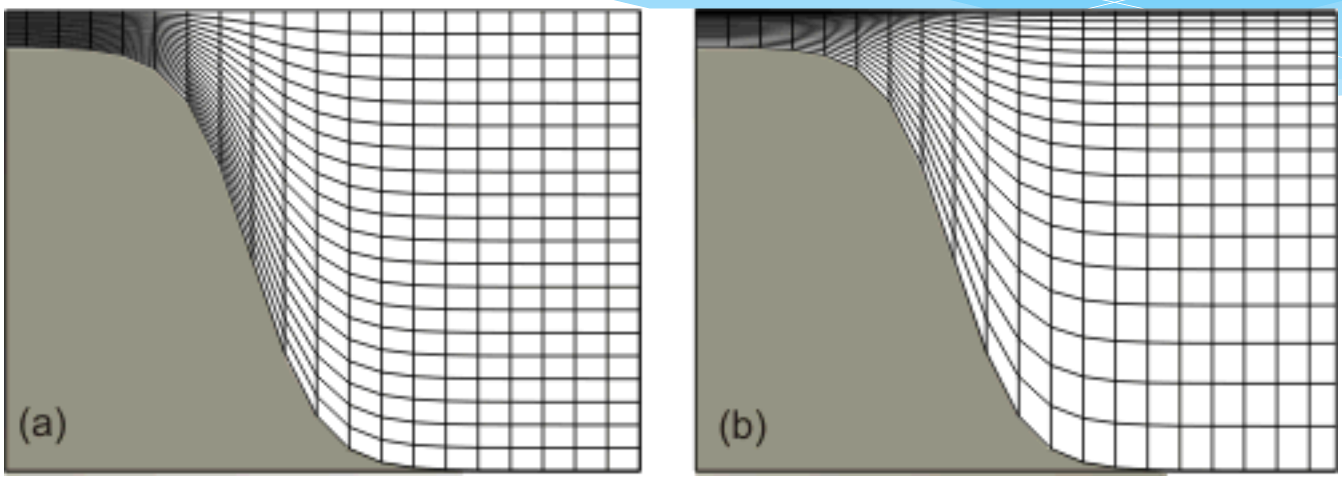
* Why does this matter for ocean DA?
  * The higher the resolution, the more expensive the model.
  * 4DVar needs iterations, EnKF requires an ensemble and accurate error covariances.

Vertical discretisation



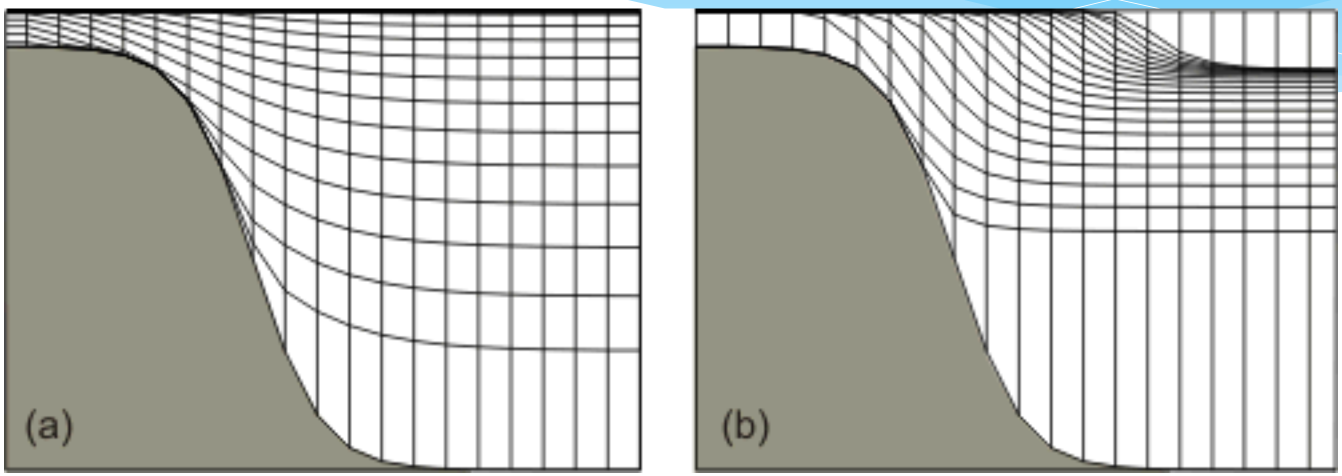
* Z-coordinate
* ++ Simple representation of gravity forces (along z)
* - - Difficult representation of lateral boundaries
* Models: NEMO, MITgcm, MOM (GFDL)

Vertical discretisation



* Sigma-coordinate (terrain following)
* ++ Continuity of the bottom layer
* - - Coarse approximation in the horizontal gradient of pressure
* Models: ROMS

Vertical discretisation



* Isopycnic coordinate
* ++ Representation of isopycnal diffusion
* - - Poor performance in weakly stratified regions
* Models: HYCOM (though hybrid in practice)

Vertical discretisation

* Why does this matter for ocean DA?
  * Most observations provide surface information.
  * The way this information penetrates in the deep ocean is essential for DA's performance.

Uncertainties

* Unresolved scales and parameterizations
* Forcings and boundary conditions

Uncertainties due to unresolved scales and parameterizations

* Dynamics at scales smaller than the grid mesh are not resolved explicitly.
* Their effect on larger scales can be parameterized, or ignored.

Uncertainties due to unresolved scales and parameterizations

* Lateral mixing due to turbulence
* Vertical mixing
* Convection
* …

Uncertainties due to unresolved scales and parameterizations

* Examples of parameterizations for vertical mixing:
  * Second-moment closure models (many exist)
  * Pacanowski and Philander (1981)
  * Mellor and Yamada (1982)
  * TKE (Turbulent Kinetic Energy), Blanke and Delecluse (1993)
  * Kraus and Turner (1967)
  * K-Profile Parameterization (KPP), Large et al. (1994)

Uncertainties due to unresolved scales and parameterizations

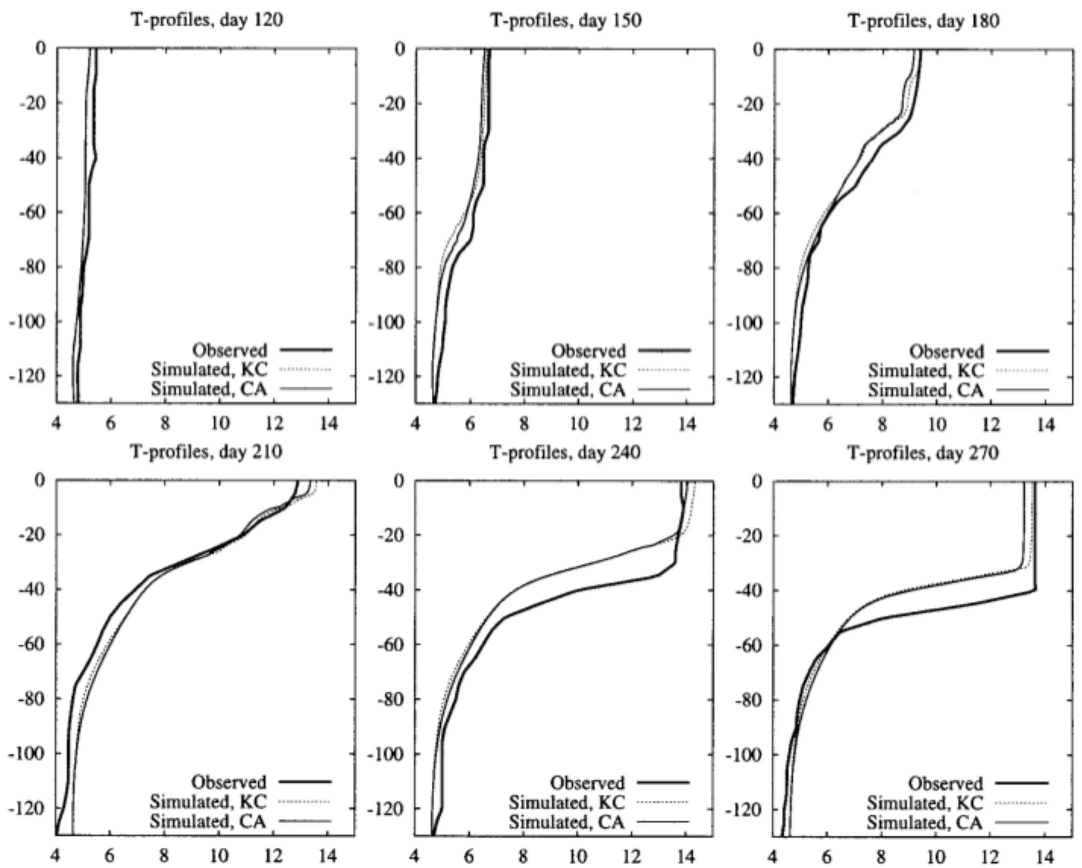


FIG. 18. Measured and simulated temperature profile at station OWS Papa during spring and summer 1961. The simulations were carried out with the quasi-equilibrium version of the Kantha and Clayson (1994) model with the stationary gradient Richardson number set to $R_i^{st} = 0.225$ and the version A of the Canuto et al. (2001) model with the stationary gradient Richardson number set to $R_i^{st} = 0.25$.

(Burchard and Bolding, 2001)

Ocean models

Uncertainties due to unresolved scales and parameterizations

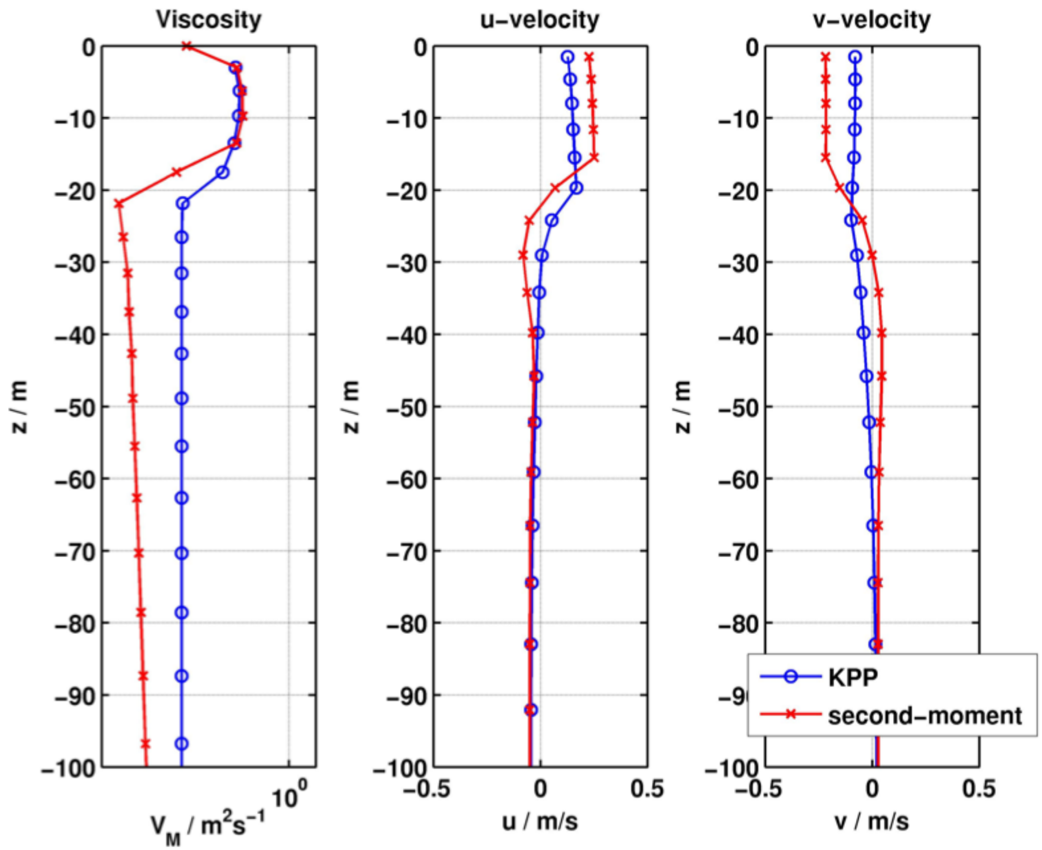


Fig. 12. Eddy viscosity and u and v velocity components from simulations in the LV station on 5 August 2004.

(Fernandez et al., 2006)

Uncertainties due to unresolved scales and parameterizations

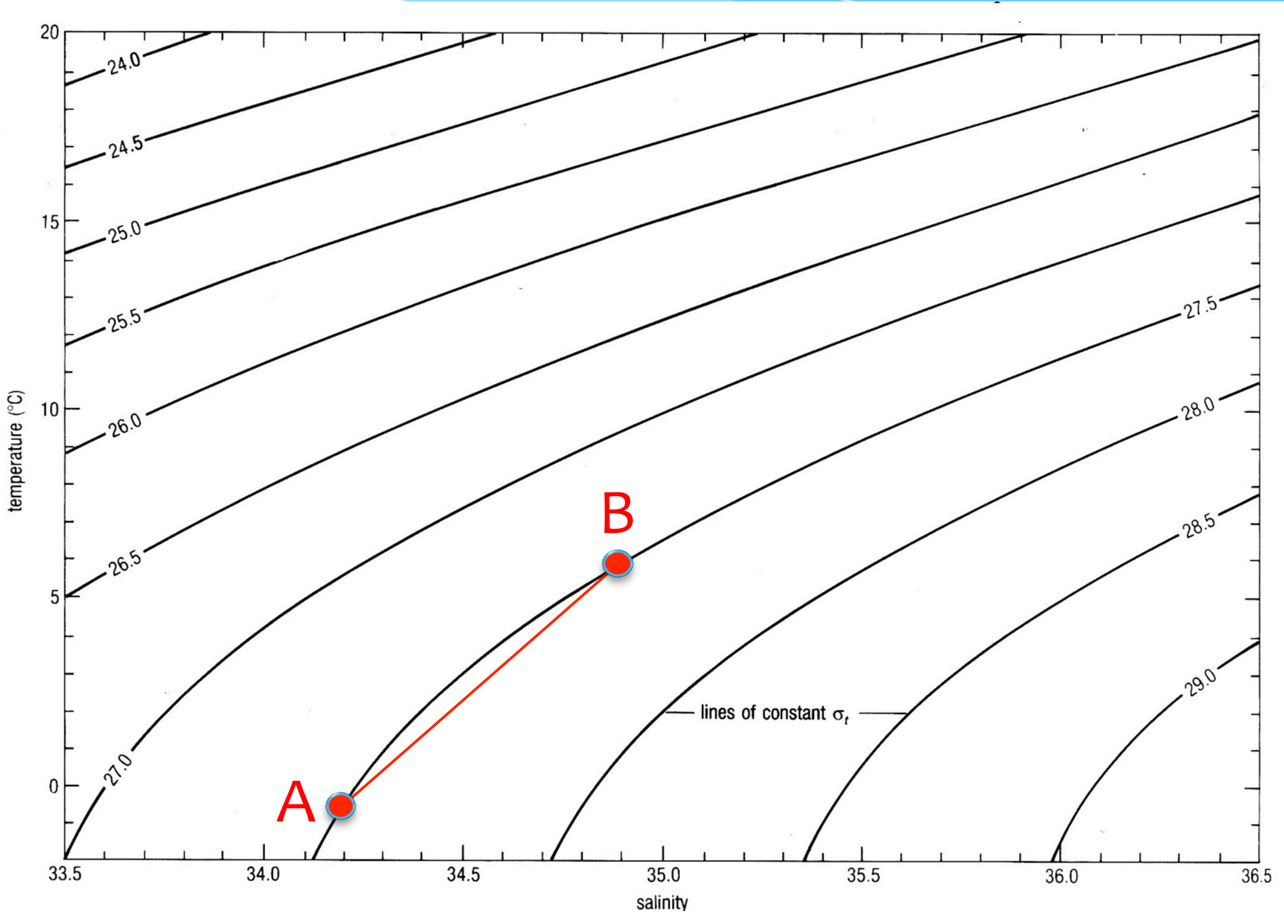
* Example of (generally) ignored effect: the state equation
  * Let <A> be the average value of A in the model gridpoint;
  * The model computes <T>, <S> from the conservation equations
  * Then compute density as:

$$\rho = \rho(< T >, < S >)$$

* Which is different from:

$$\rho =< \rho(T, S) >$$

Uncertainties due to unresolved scales and parameterizations

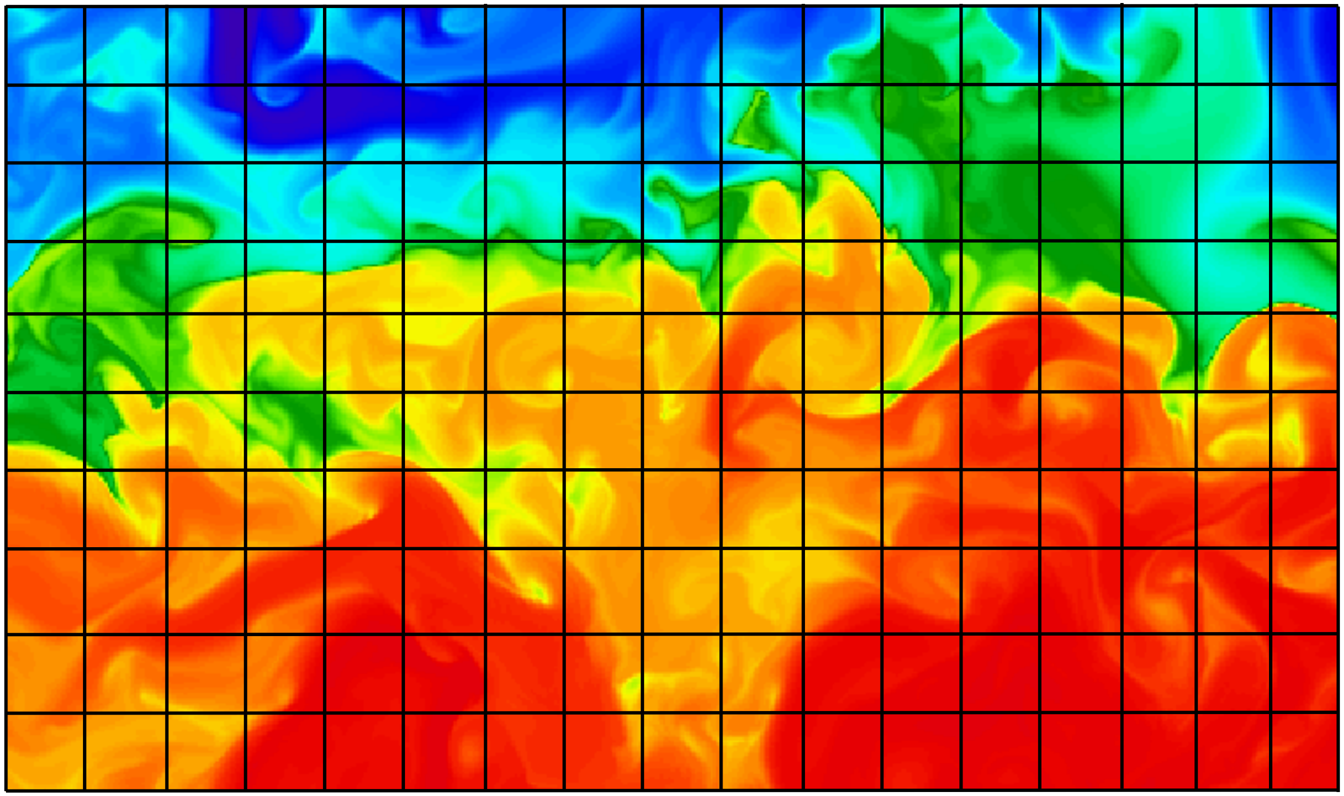


$$\rho(A+B) \neq \rho(A) + \rho(B)$$

Ocean models

Uncertainties due to unresolved scales and parameterizations

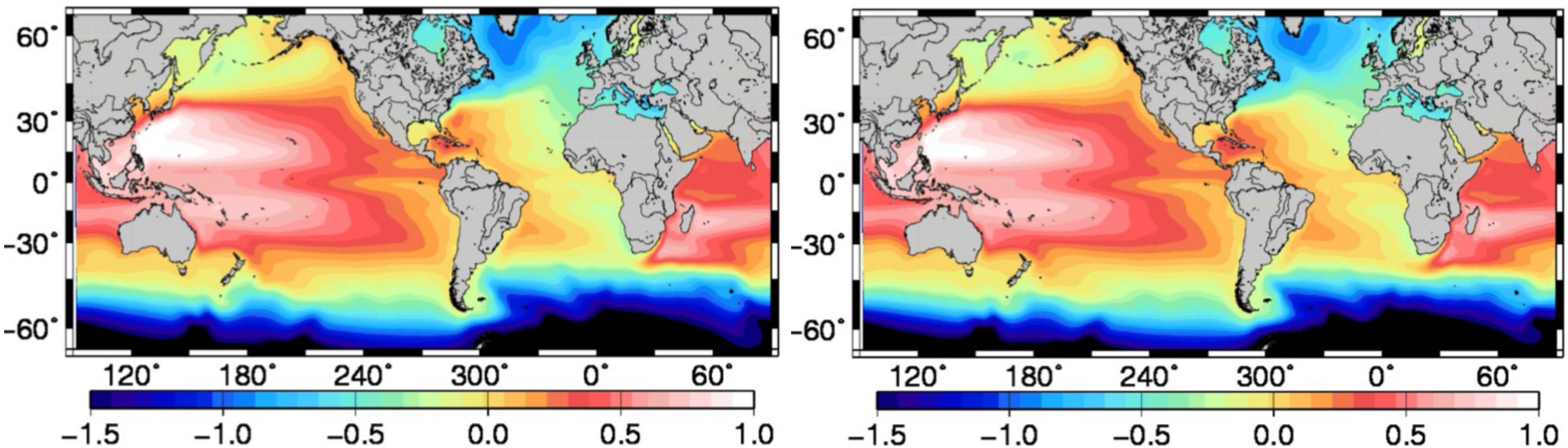
A realistic temperature field and a possible model grid



Uncertainties due to unresolved scales and parameterizations

Fields of SSH from NEMO, ORCA2 (gridmesh 2°)

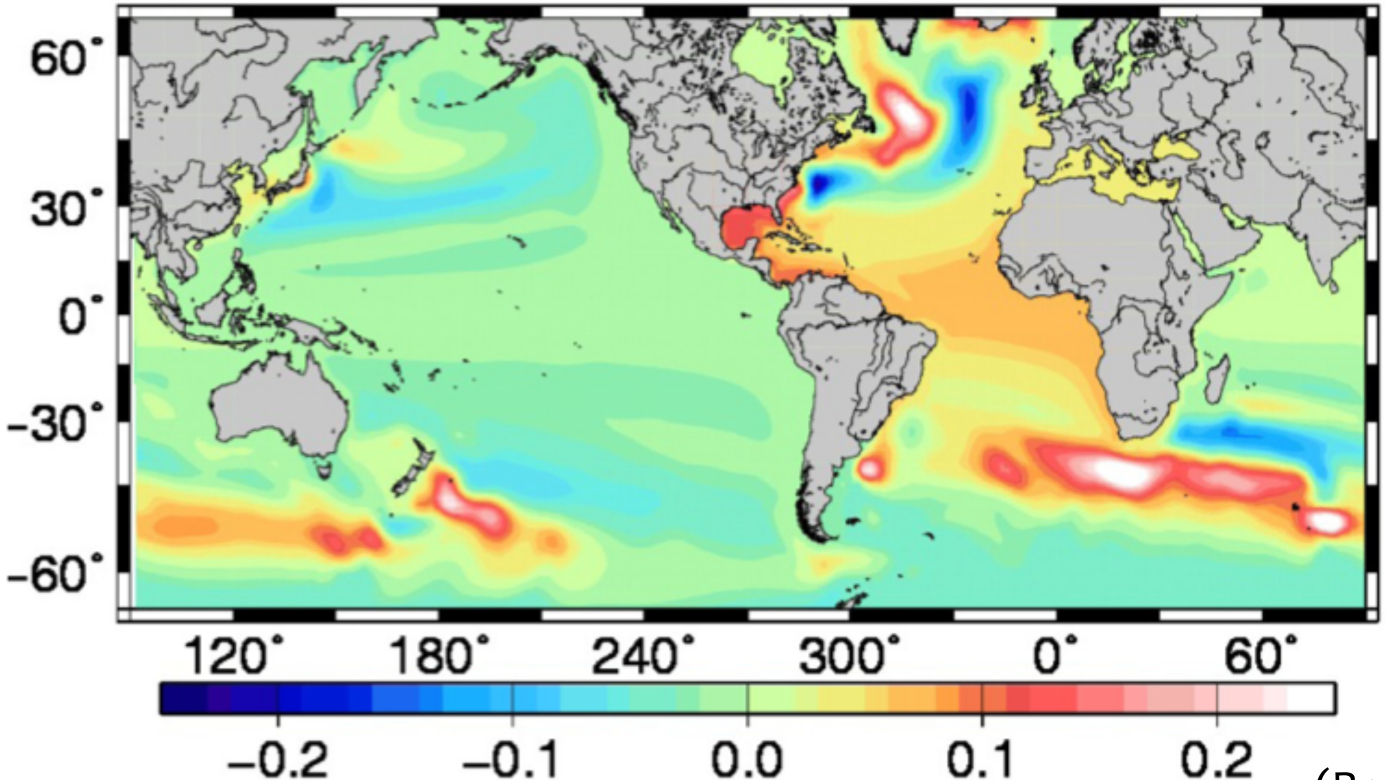
$$\rho = \rho(< T >, < S >) \qquad \rho = < \rho(T, S) >$$



(Brankart, 2013)

Uncertainties due to unresolved scales and parameterizations

Difference

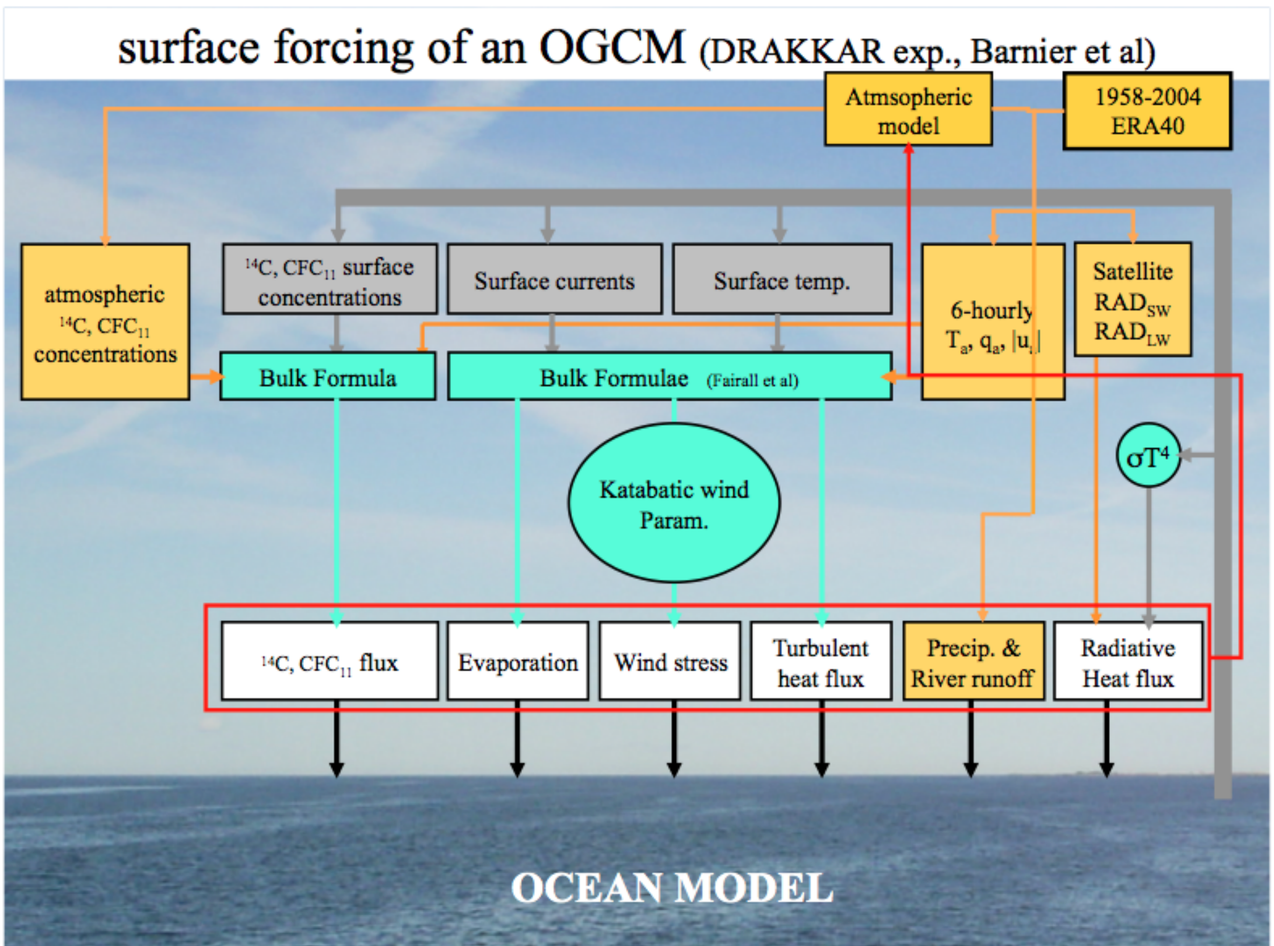


(Brankart, 2013)

Uncertainties due to boundary conditions

* Ocean models are forced at their surface by atmospheric fluxes: winds, mass and heat fluxes;
* They are influenced by the bottom surface and bathymetry, continents, islands;
* Regional models are driven at their open boundaries.

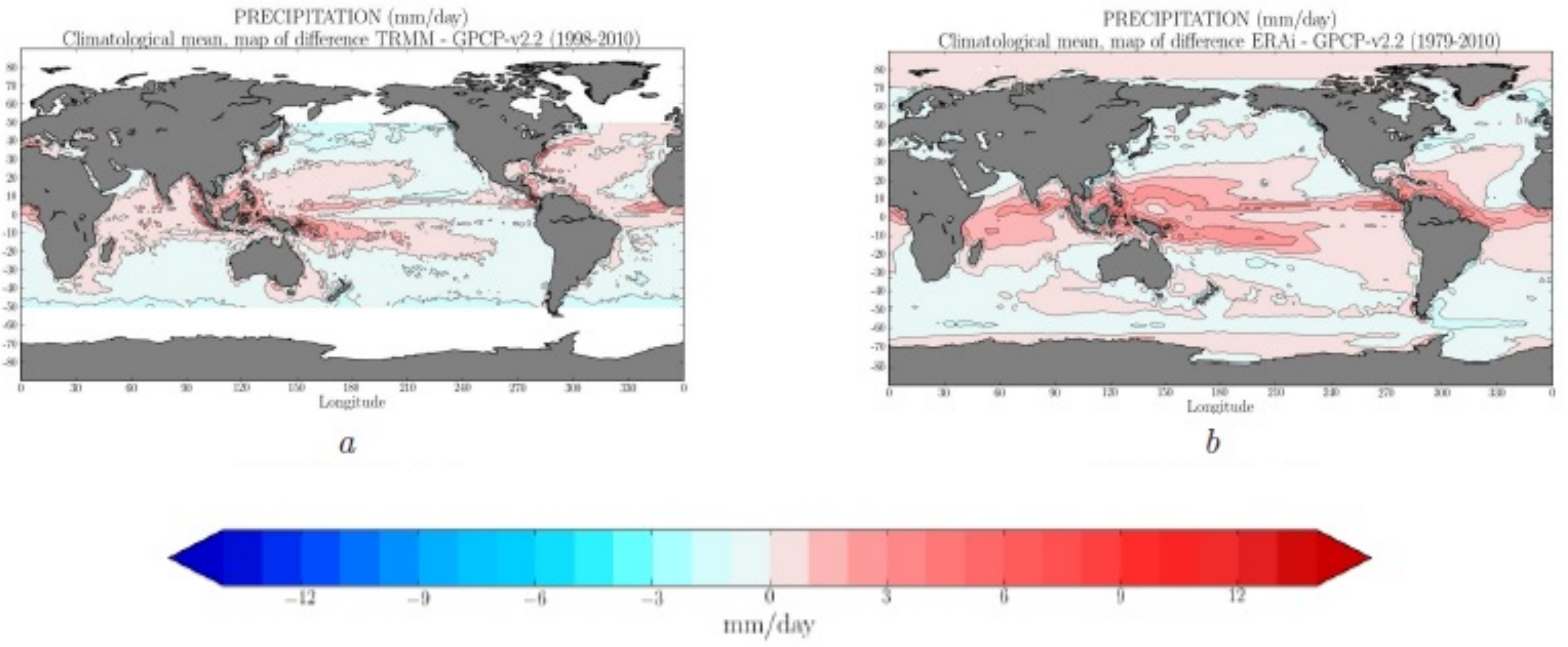
Uncertainties due to boundary conditions



Yellow: atmospheric
Grey: oceanic
Green: parameterizations
White: physical processes

Ocean models

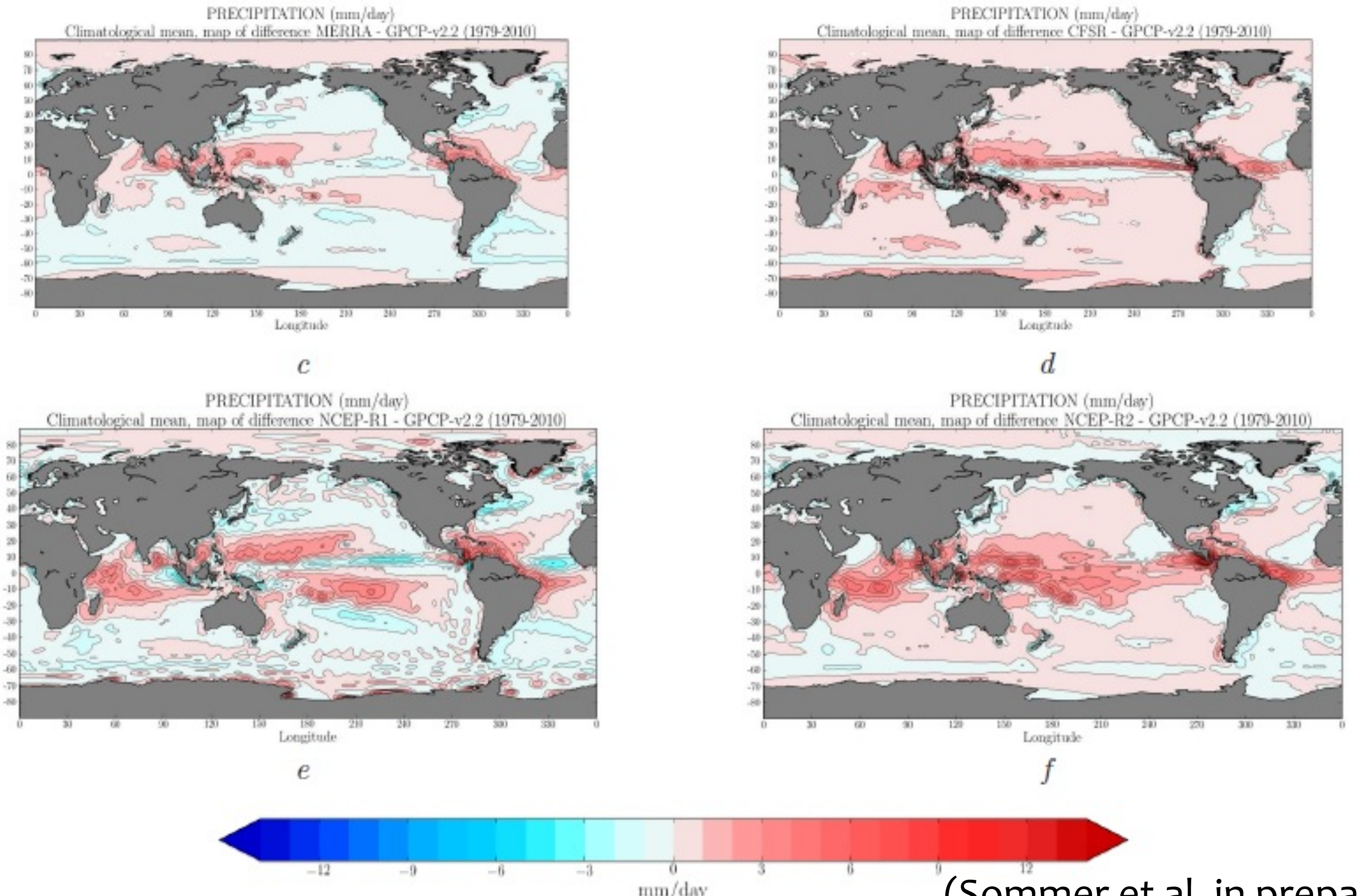
Uncertainties due to boundary conditions



(Sommer et al, in preparation)

Ocean models

Uncertainties due to boundary conditions



(Sommer et al, in preparation)

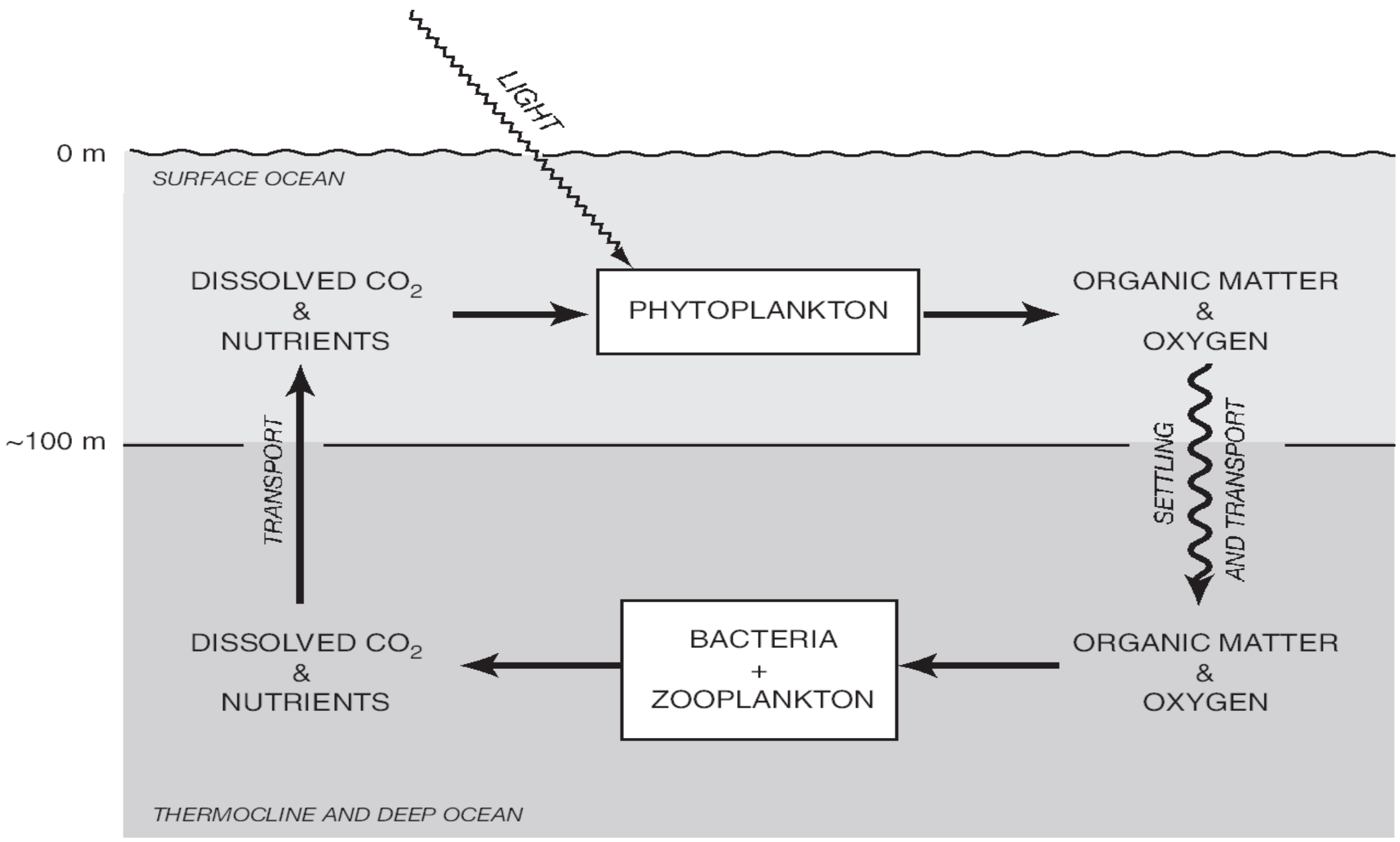
Uncertainties due to boundary conditions

* Lateral boundary conditions: free slip, partial slip, no slip;
* Bottom friction: quadratic with a drag coefficient, or no friction;
* Open boundary conditions come from climatologies or other model simulations.

Ocean models: uncertainties

* Why does this matter for ocean DA?
  * Models has many sources of uncertainty;
  * To provide the best representation of the ocean state, models must be constrained by observations with DA;
  * To set up the DA system correctly, one must identify at best the various sources of errors and parameterize their impact;
  * DA can "guide" models, but also help in reducing the original uncertainties (e.g., by estimating parameters)

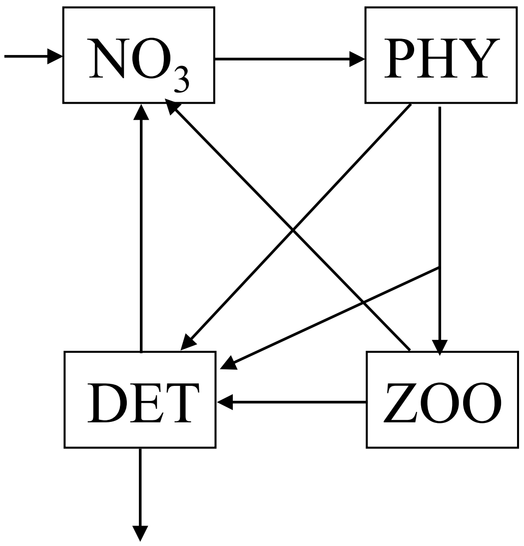
Biogeochemistry



Ocean primary production is a key piece of the ocean life and the carbon cycles.

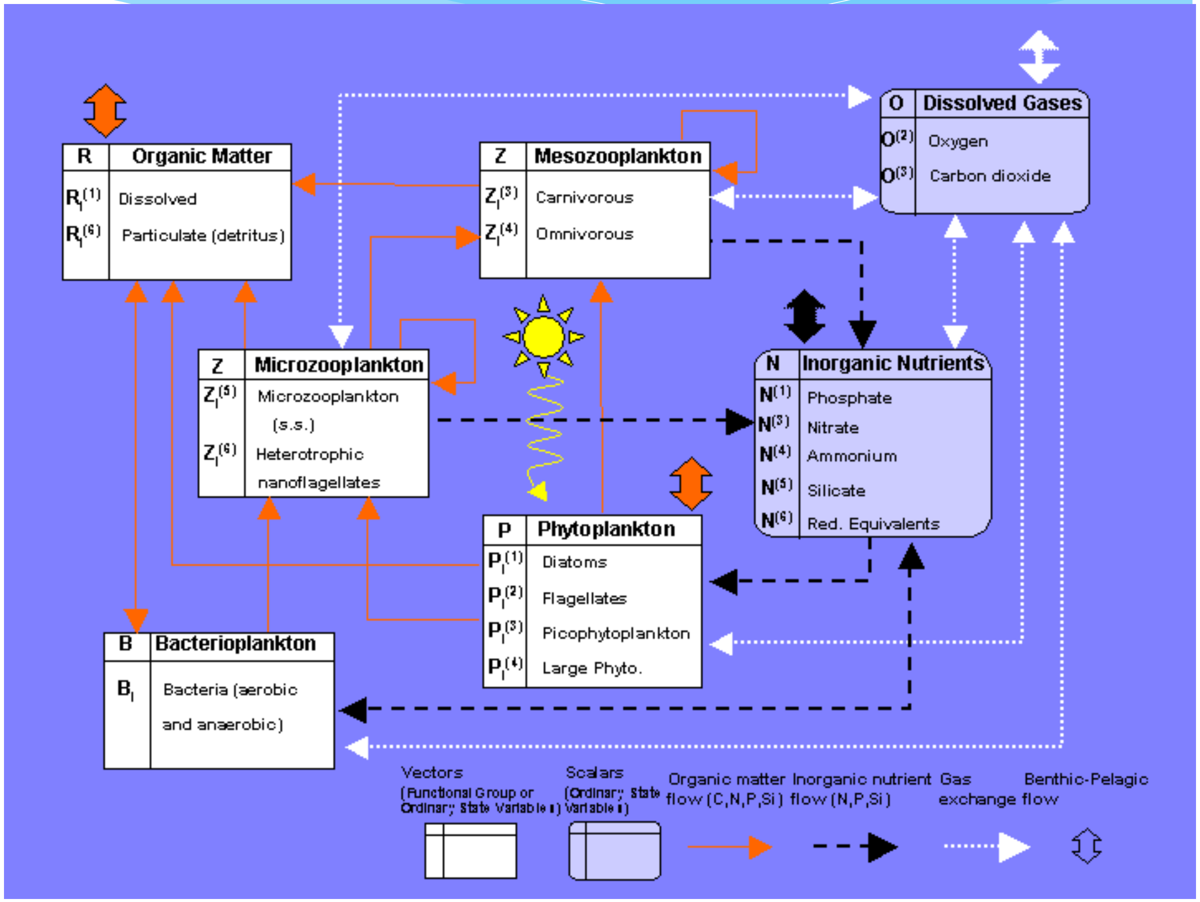
Biogeochemistry

- Simple NPZD ecosystem model (Nutrients, Phyto, Zoo, Detritus)
- 10-30 tunable parameters:
  - Growth rate, mortality
  - Sedimentation speed
  - Etc
- Already challenging for assimilation



Biogeochemistry

* Generic pelagic ecosystem models
* More than 100 tunable parameters



(Vichy et al, 2007)

Biogeochemistry

❑ Hydrodynamics

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}.\nabla^h \boldsymbol{u} + w\frac{\partial \boldsymbol{u}}{\partial z} + fe_z \Lambda \boldsymbol{u} = -\frac{1}{\rho}\nabla^h p + \frac{\partial}{\partial z}\left(\tilde{\upsilon}\frac{\partial \boldsymbol{u}}{\partial z}\right) + D(\boldsymbol{u})$$

$$\nabla^h.\boldsymbol{u} + \frac{\partial w}{\partial z} = 0$$

$$\frac{\partial T}{\partial t} + \boldsymbol{u}.\nabla^h T + w\frac{\partial T}{\partial z} = \frac{\partial}{\partial z}\left(\tilde{\lambda}\frac{\partial T}{\partial z}\right) + Q(T)$$

$$\frac{\partial S}{\partial t} + \boldsymbol{u}.\nabla^h S + w\frac{\partial S}{\partial z} = \frac{\partial}{\partial z}\left(\tilde{\lambda}\frac{\partial S}{\partial z}\right)$$

$$\frac{\partial p}{\partial z} = -\rho g \qquad (\tilde{\upsilon},\tilde{\lambda}) = f\left(\frac{\partial \rho}{\partial z},\frac{\partial \boldsymbol{u}}{\partial z}\right)$$

c_i

Physical state uncertainties: vertical advective/diffusive fluxes

$$\boldsymbol{u}\,,\, w\,,\, \tilde{\lambda}$$

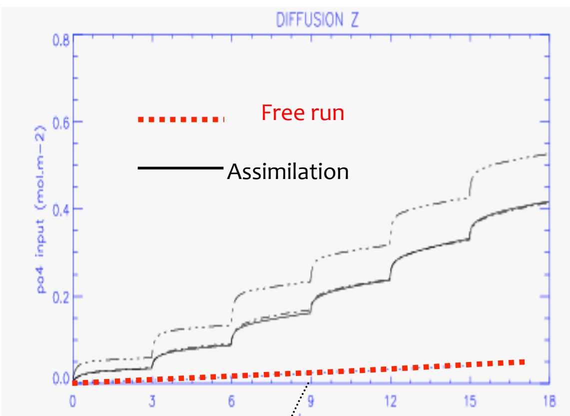
Parameter uncertainties: biological interactions

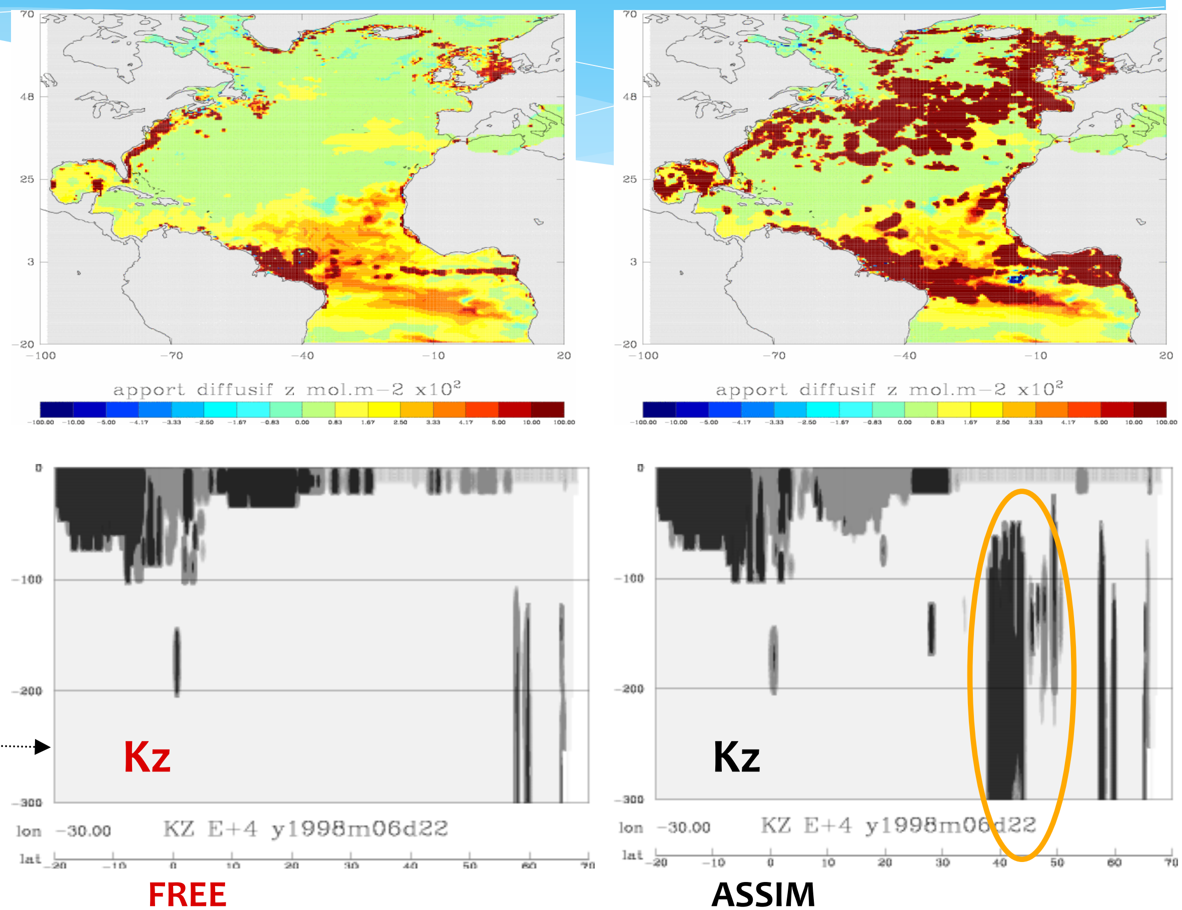
Biological state uncertainties: surface and deep stocks

❑ Biology

$$\frac{\partial c_i}{\partial t} + \boldsymbol{u}.\nabla^h c_i + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial z}\left(\tilde{\lambda}\frac{\partial c_i}{\partial z}\right) + S(c_i, c_j, \alpha_n) \quad i = 1, N$$

Biogeochemistry





* An "bad" assimilation in the dynamics can be detrimental to biology

(Berline et al, 2005)

Biogeochemistry

* No basic rule (e.g., Navier-Stokes equations) for biology
* Many uncertain and tunable parameters
* Biology sensitive to dynamics and dynamical instabilities
* Tracer concentrations are positive variables

Ocean models: summary

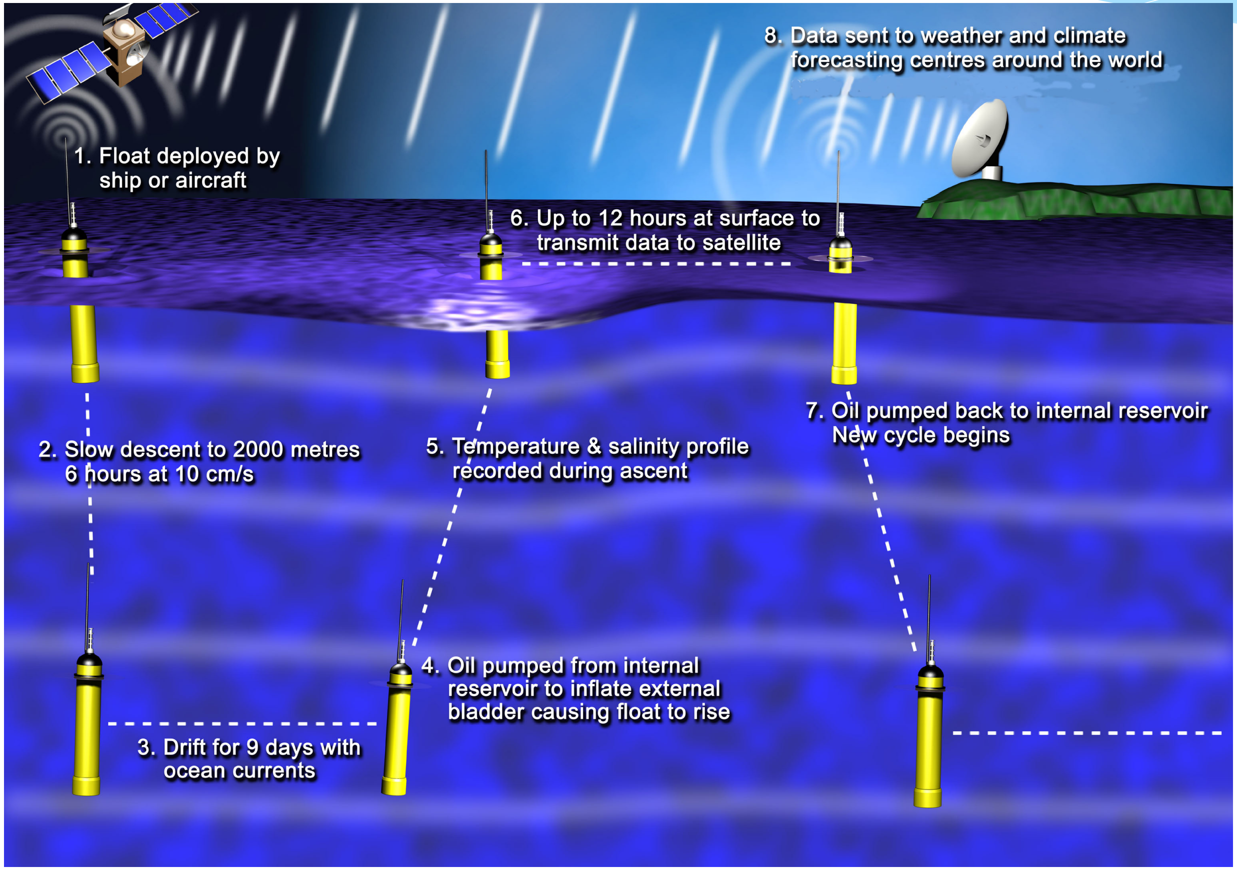
* Models are:
  * nonlinear,
  * Complex and expensive,
  * Subject to many uncertainties,
  * With non Gaussian variables,
  * etc

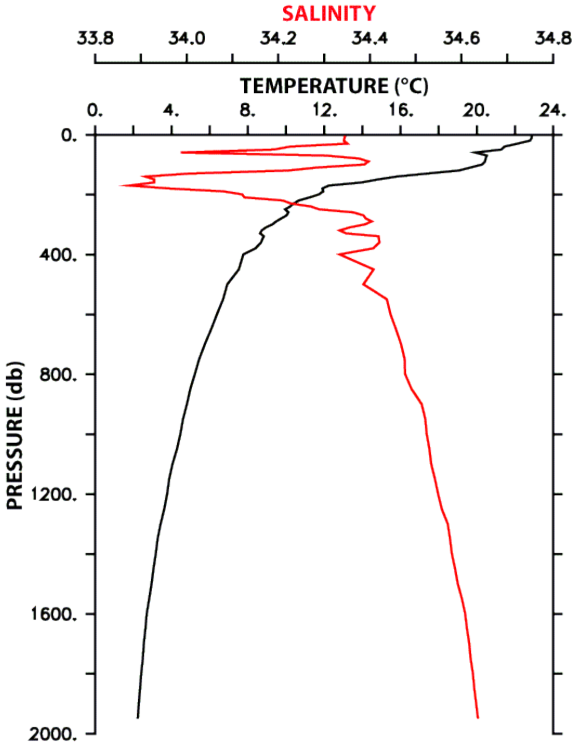
Observations

* In situ observations
  * Profiling floats: ARGO project
  * Moorings: OceanSITES project
  * Ships: SOOP and GOSUD projects, and WOCE program
  * Surface drifters: DBCP and E-SURFMAR projects
  * Gliders: EGO initiative
  * Marine mammals
* Satellite observations
  * Altimetry
  * Sea surface temperature (SST)
  * Ocean color

In situ observation #1: profiling floats

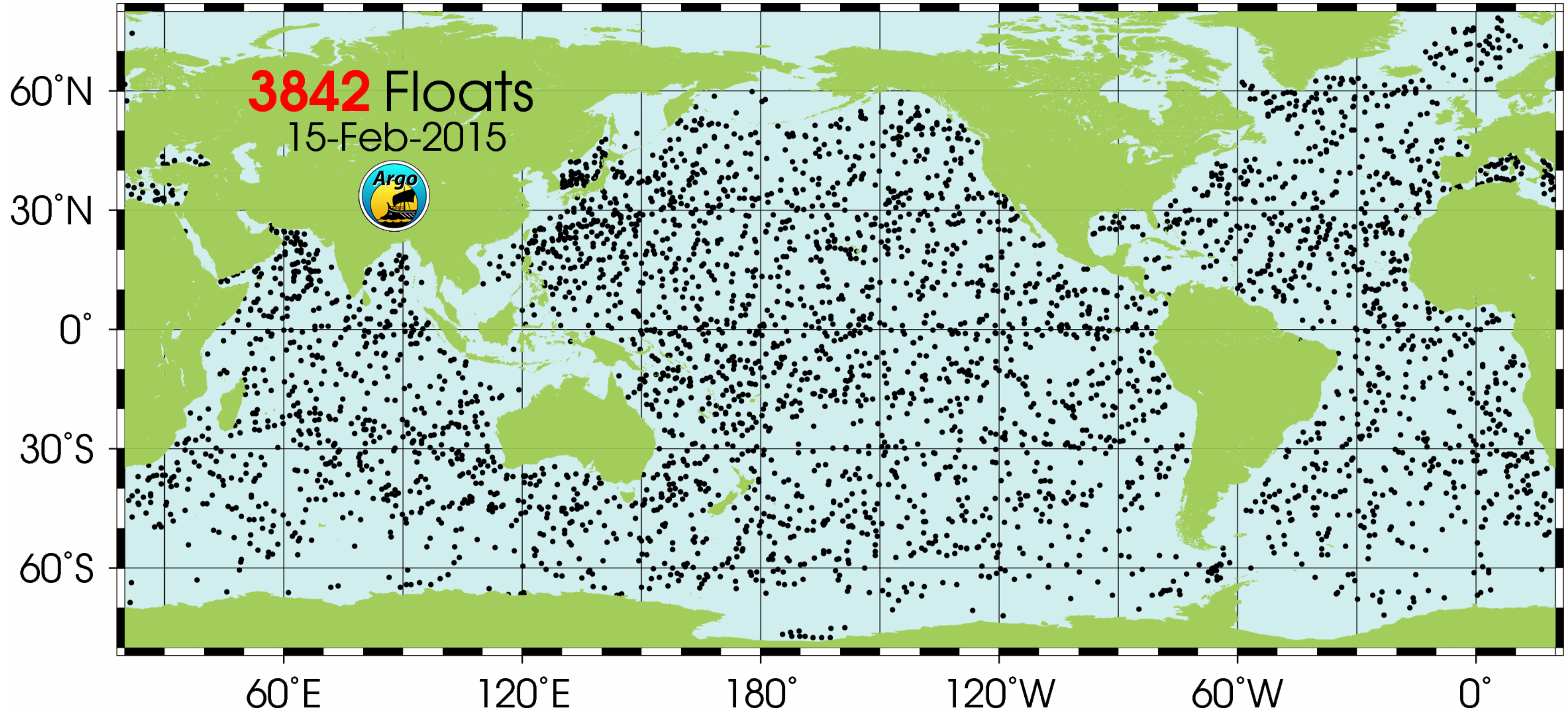
ARGO = network of profiling floats





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

In situ observation #1: profiling floats



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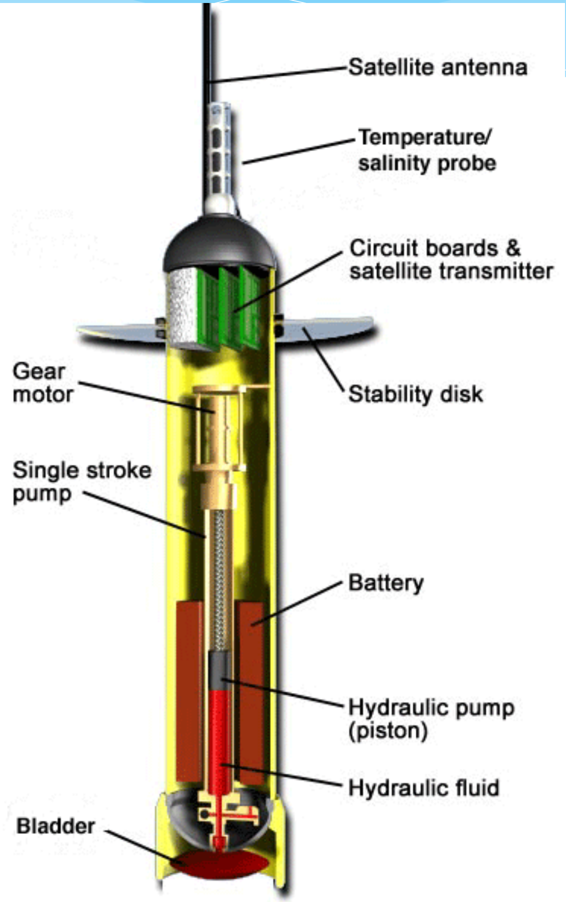
In situ observation #1: profiling floats



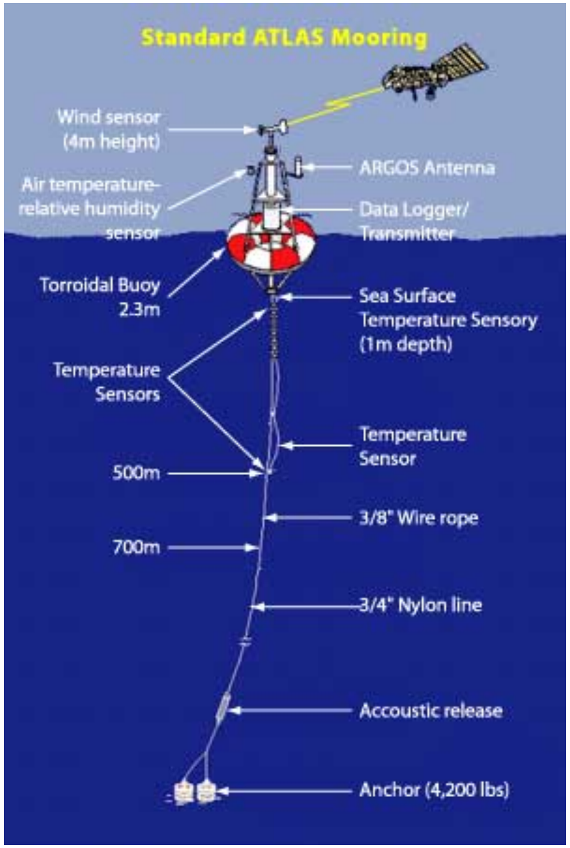
http://www.argo.ucsd.edu/

In situ observation #1: profiling floats

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

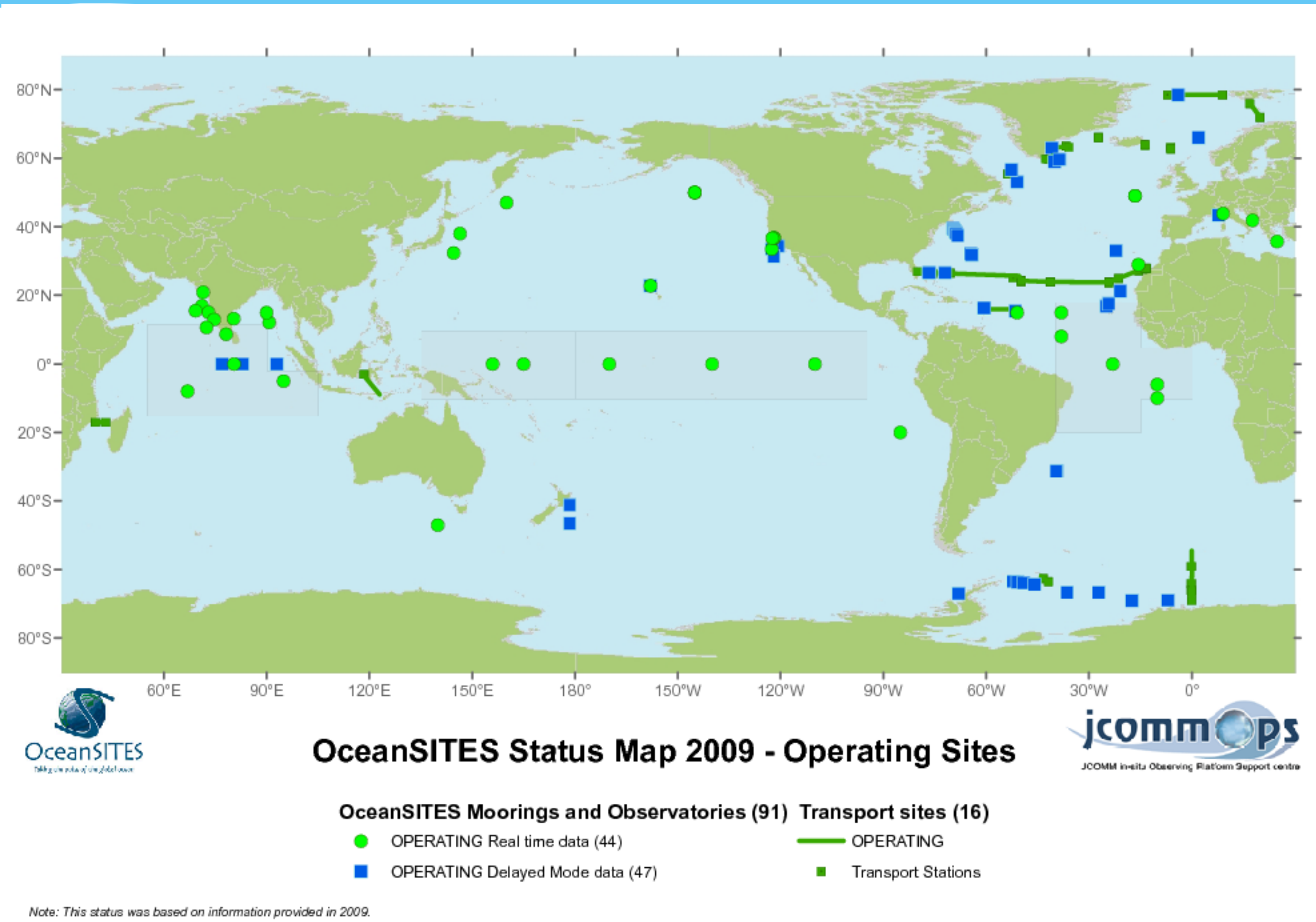
In situ observation #2: Moorings

Moorings are managed by the project OceanSITES.



Observations

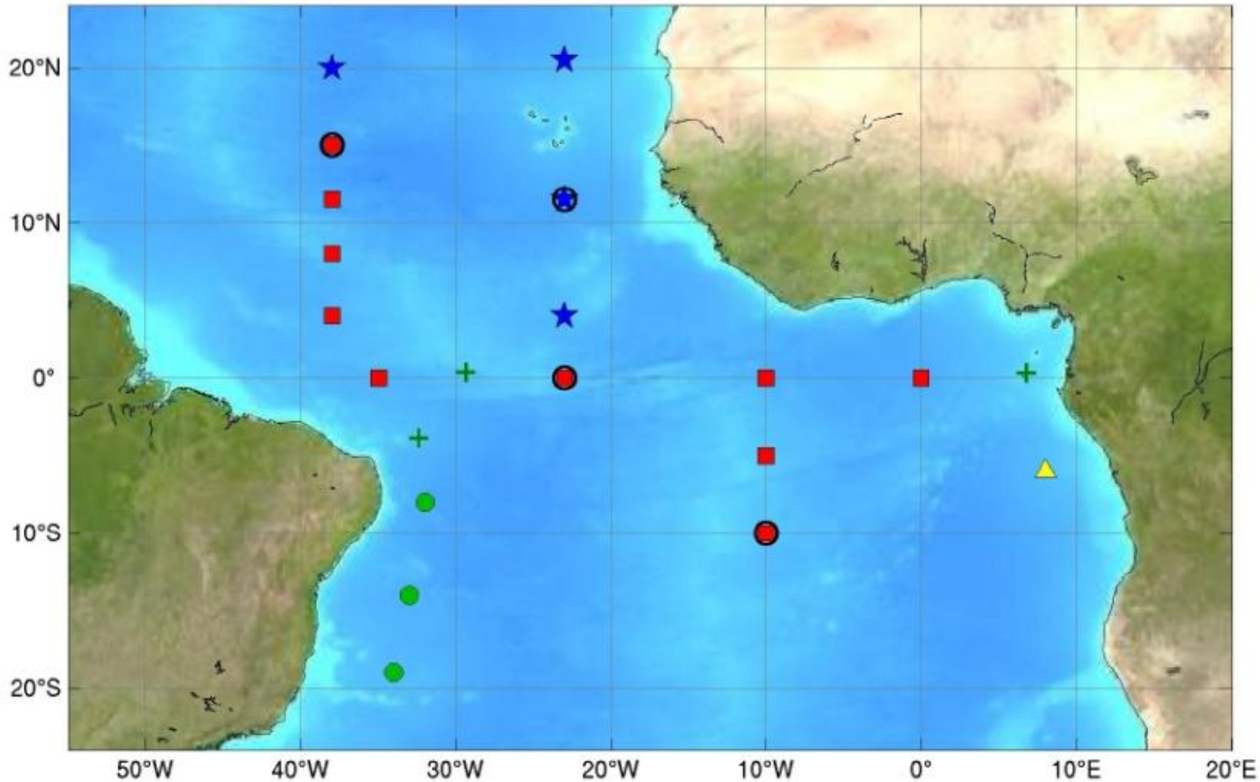
In situ observation #2: Moorings



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

In situ observation #2: Moorings

The French contribution to OceanSITES: PIRATA



http://www.brest.ird.fr/pirata/pirata.php

In situ observation #2: Moorings

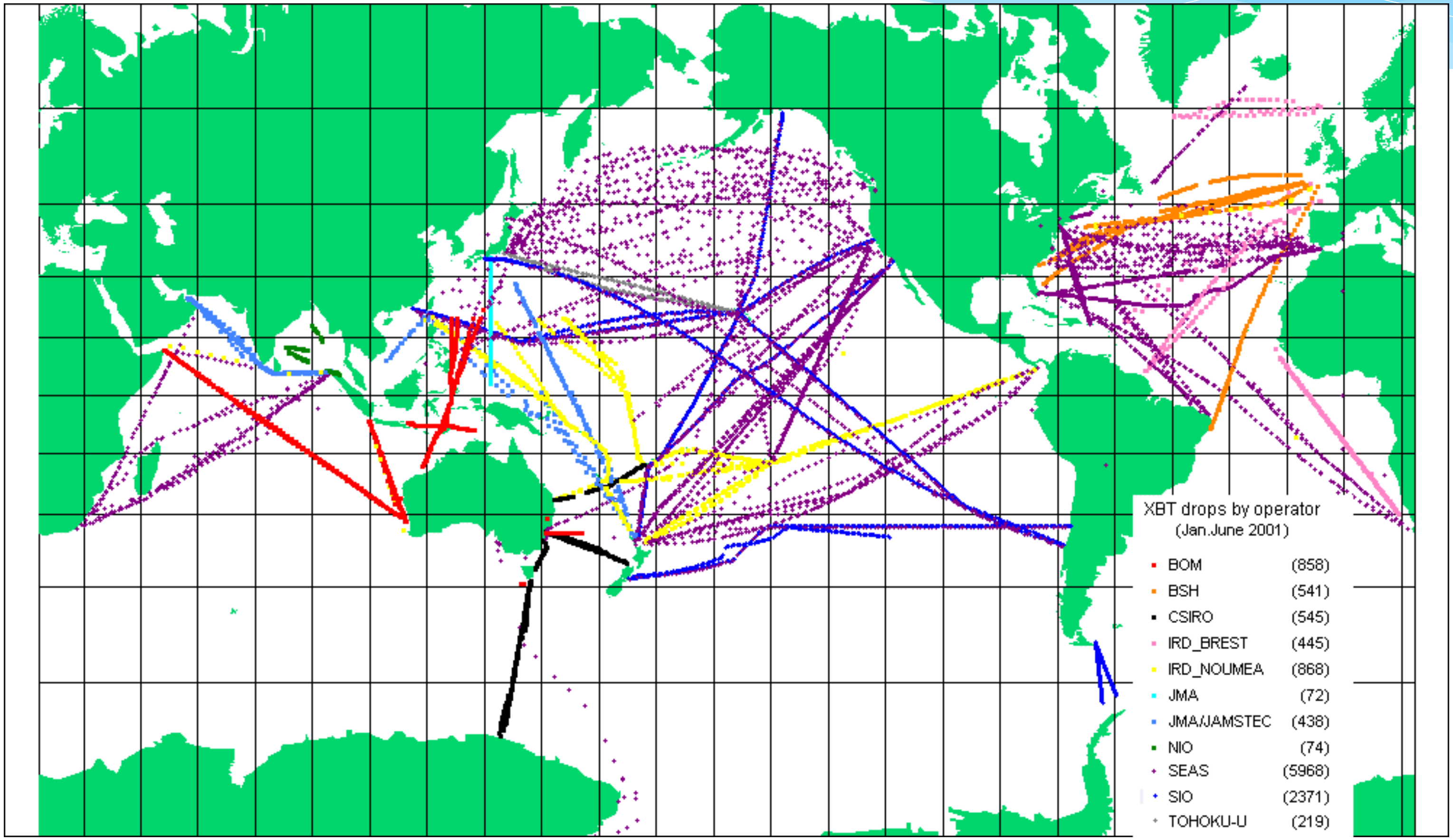
* +++ : time sampling, vertical information, autonomy
* - - - : expensive to build and maintain, poor spatial coverage

In situ observation #3: Ships

* Volunteer observing ships
* Research vessels

In situ observation #3: Ships

Ships of Opportunity: XBT drops

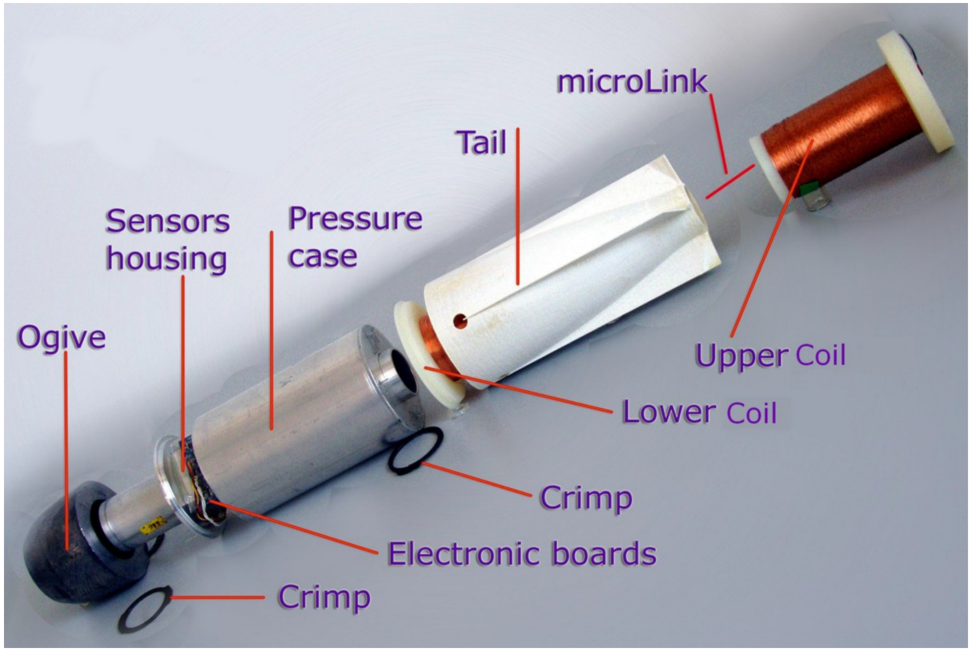


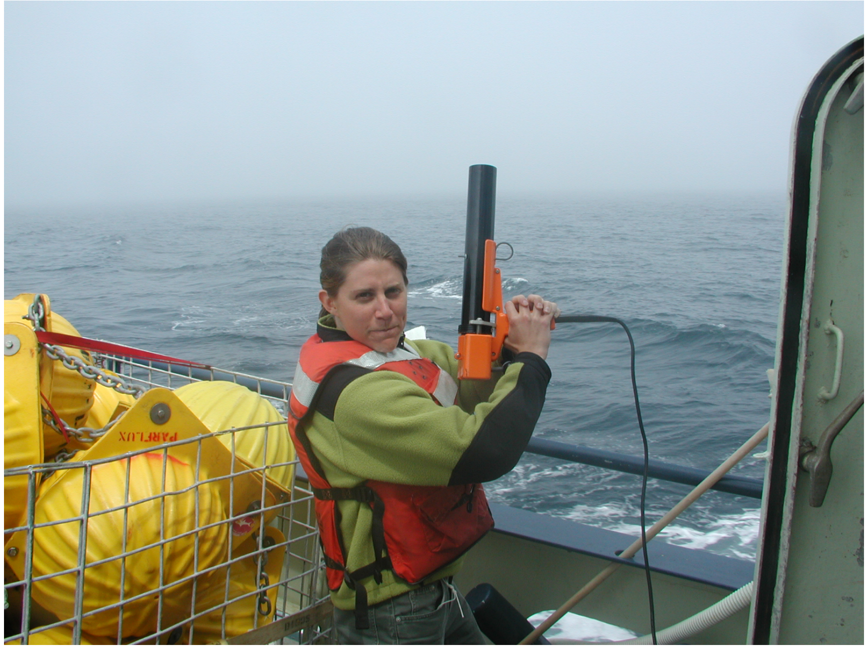
January-
June 2001

http://www.jcommops.org/soopip/

In situ observation #3: Ships

XBT probe, drop



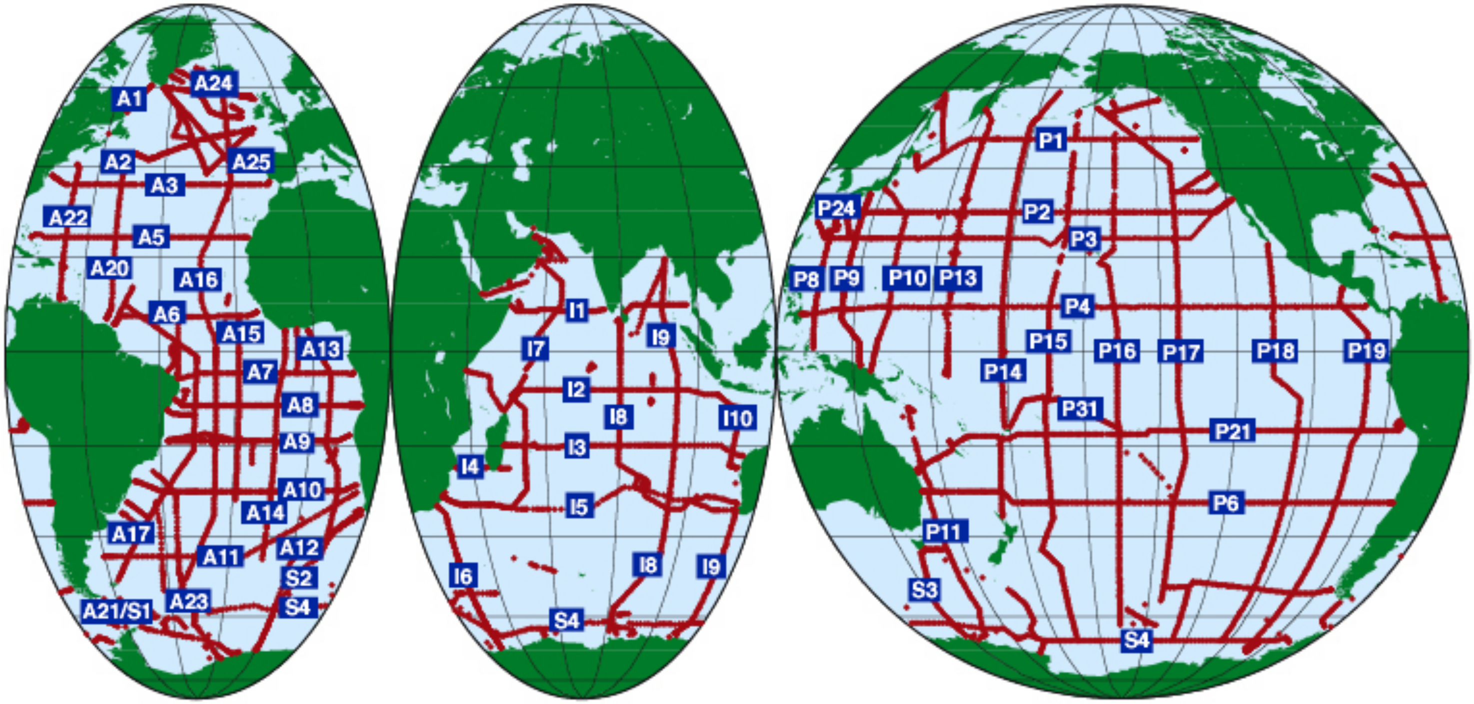


XBT: Expendable bathythermograph. Measure temperature and depth to ~1000 m

In situ observation #3: Ships

Research vessels: WOCE and isolated projects.

This survey took 10 years!



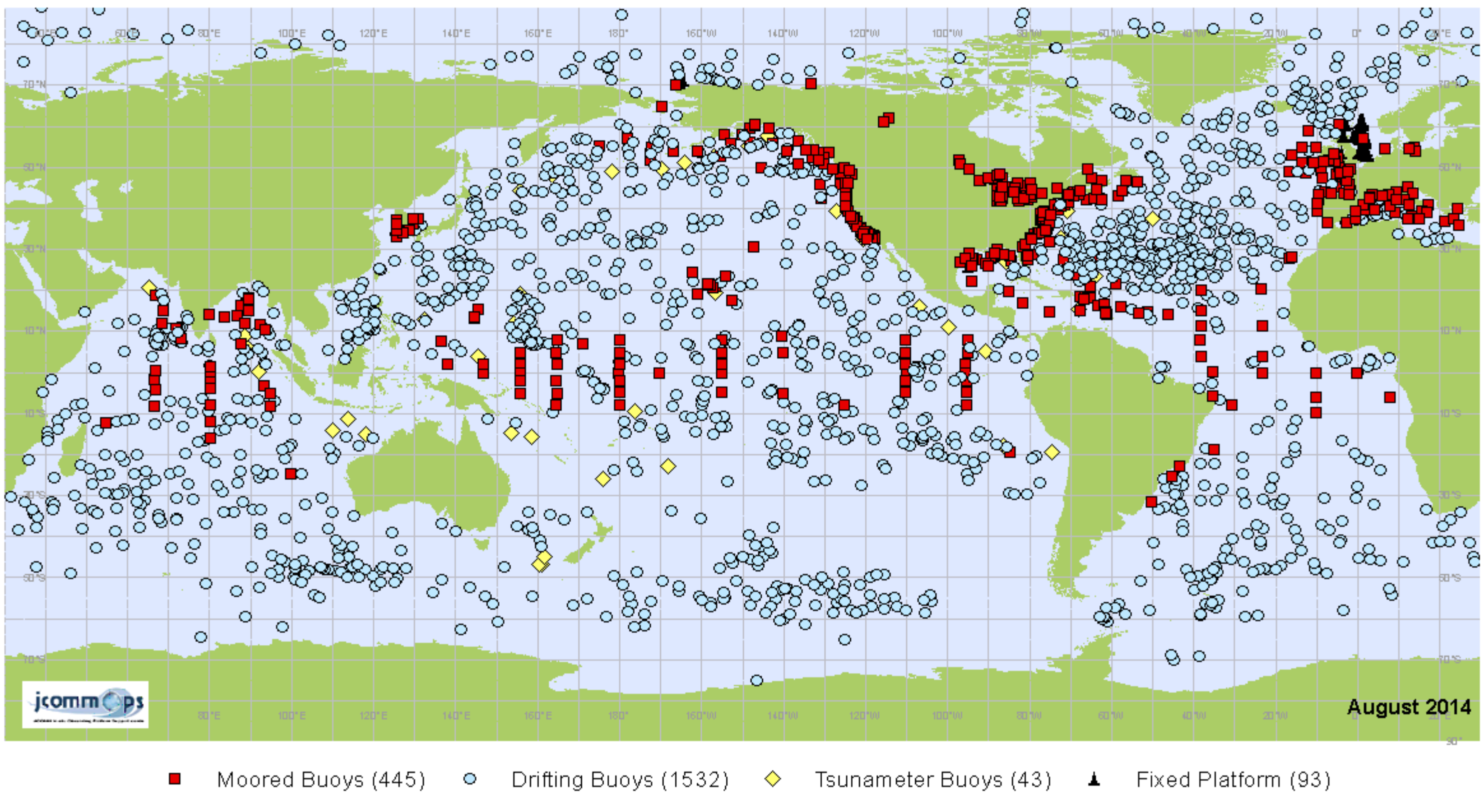
http://woceatlas.tamu.edu/

In situ observation #3: Ships

* VOS:
  * +++: cost effective, vertical information
  * - - - : limited to commercial routes, rarely deeper than 800 m
* Research vessels:
  * +++: often go to remote and poorly observed areas
  * - - - : extremely expensive, extremely poor coverage

In situ observation #4: surface drifters

Projects DBCP and E-SURFMAR



http://www.jcommops.org/dbcp/

In situ observation #4: surface drifters

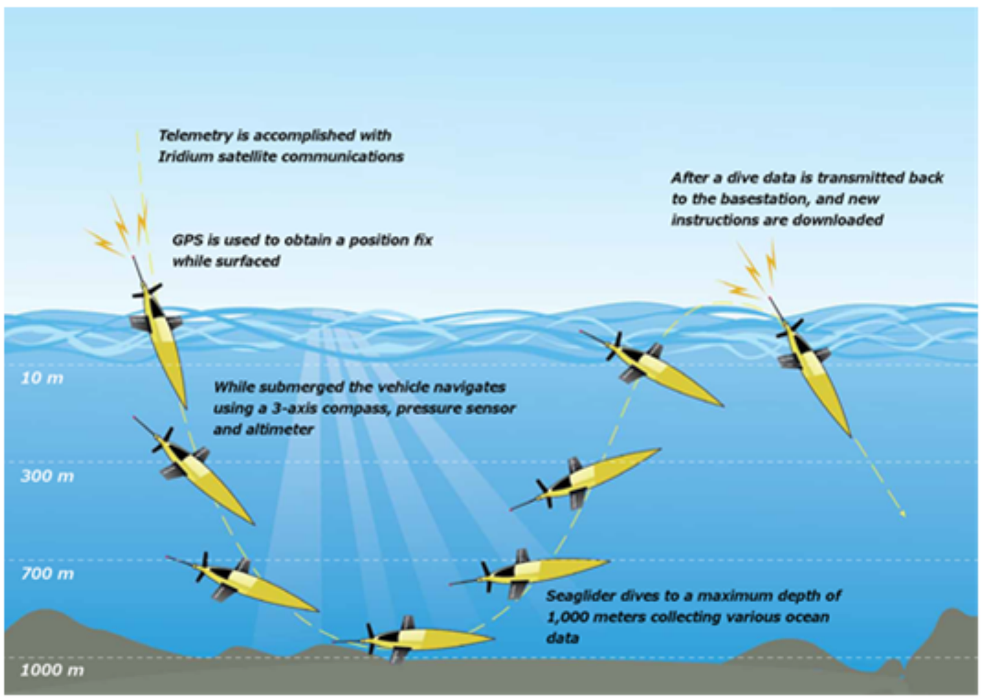
A drifter measures surface temperature and currents.
http://www.aoml.noaa.gov/
http://www.nefsc.noaa.gov/

In situ observation #4: surface drifters

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

In situ observation #5: gliders

Gliders organized within the EGO initiative



http://www.fastwave.com.au

In situ observation #5: gliders

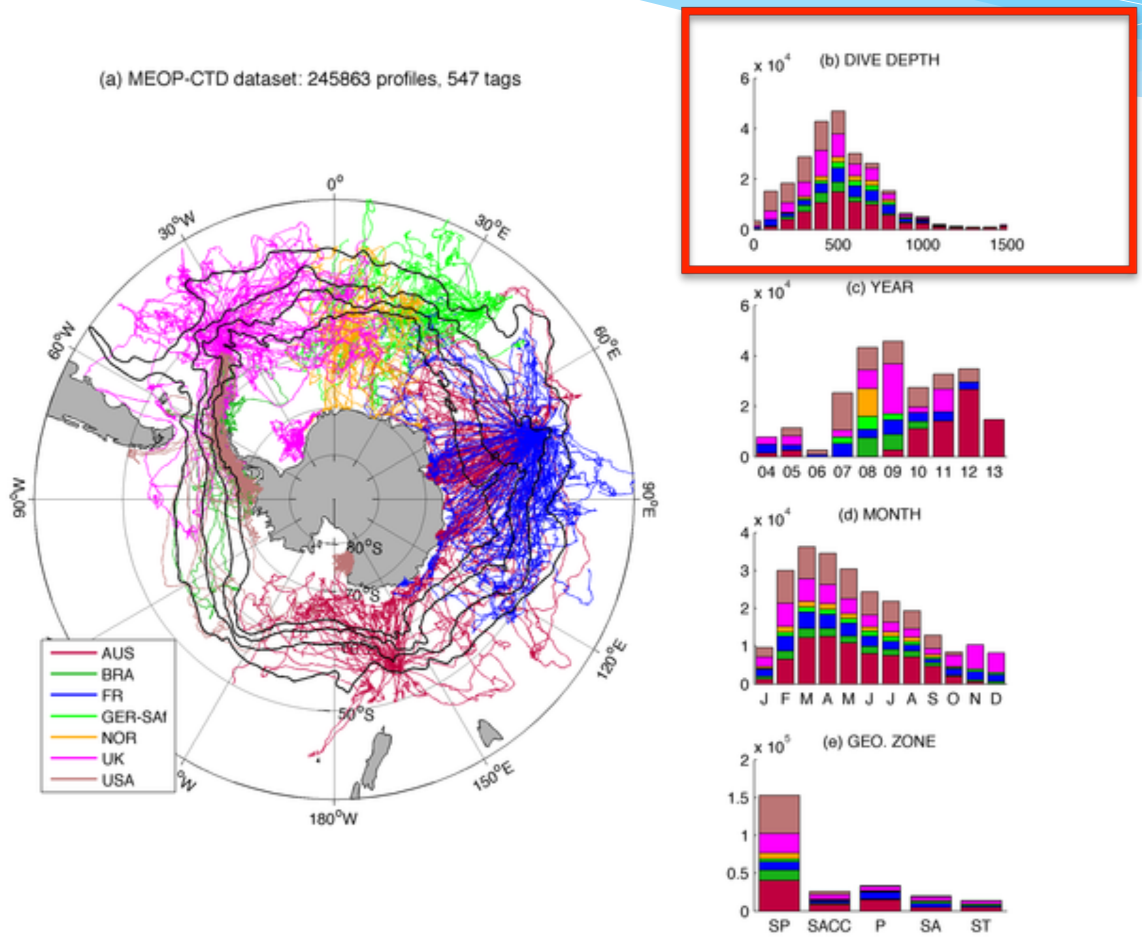
* +++: flexible, vertical information
* - - - : limited to targeted campaigns

In situ observation #6: marine mammals

A miniaturized CTD (Conductivity-Temperature-Depth) probe

Observations

In situ observation #6: marine mammals

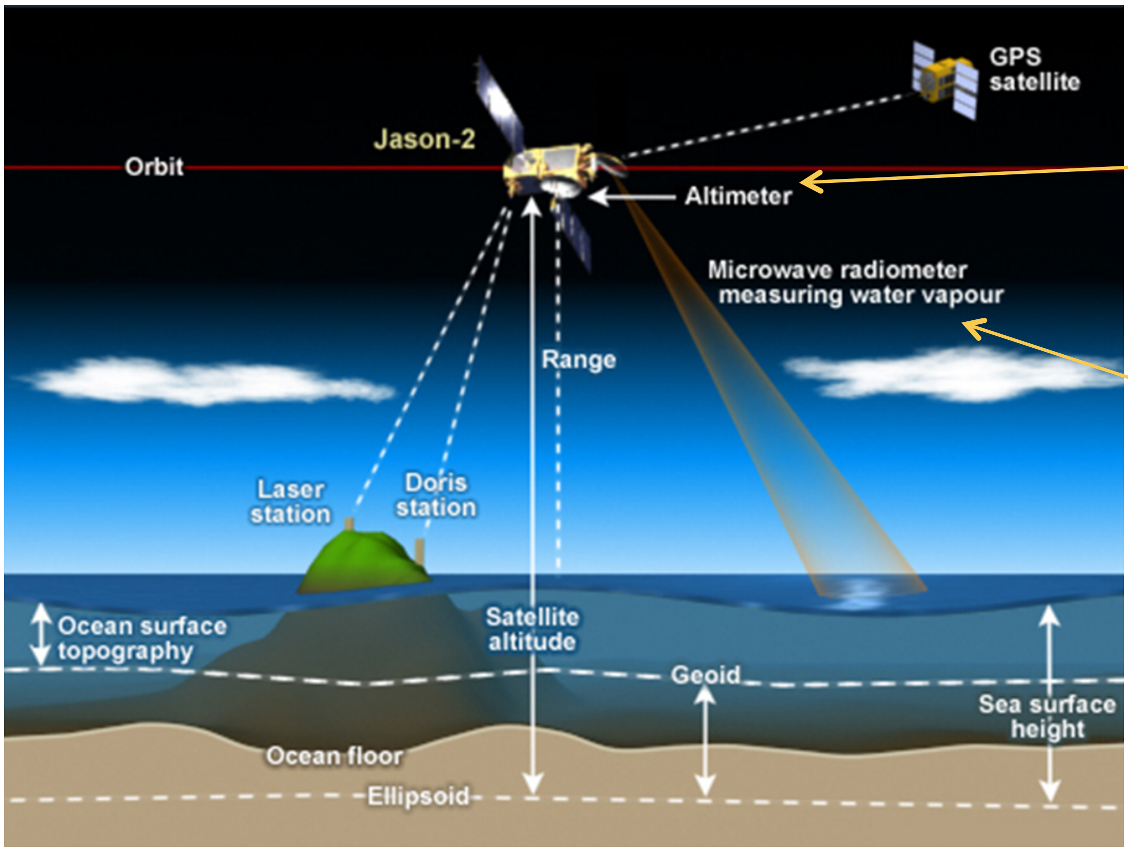


Sample poorly observed areas!

In situ observation #6: marine mammals

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

Satellite observation #1: altimetry



Radar altimeter (emitter & antenna)

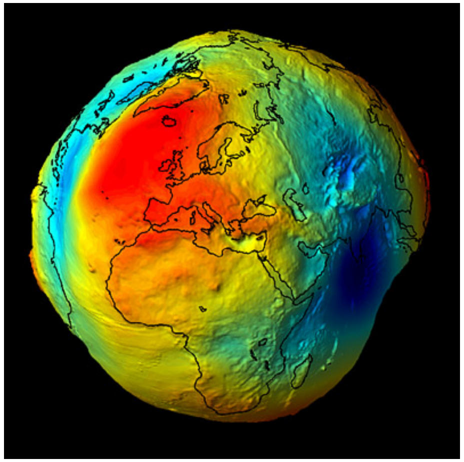
For atmospheric corrections

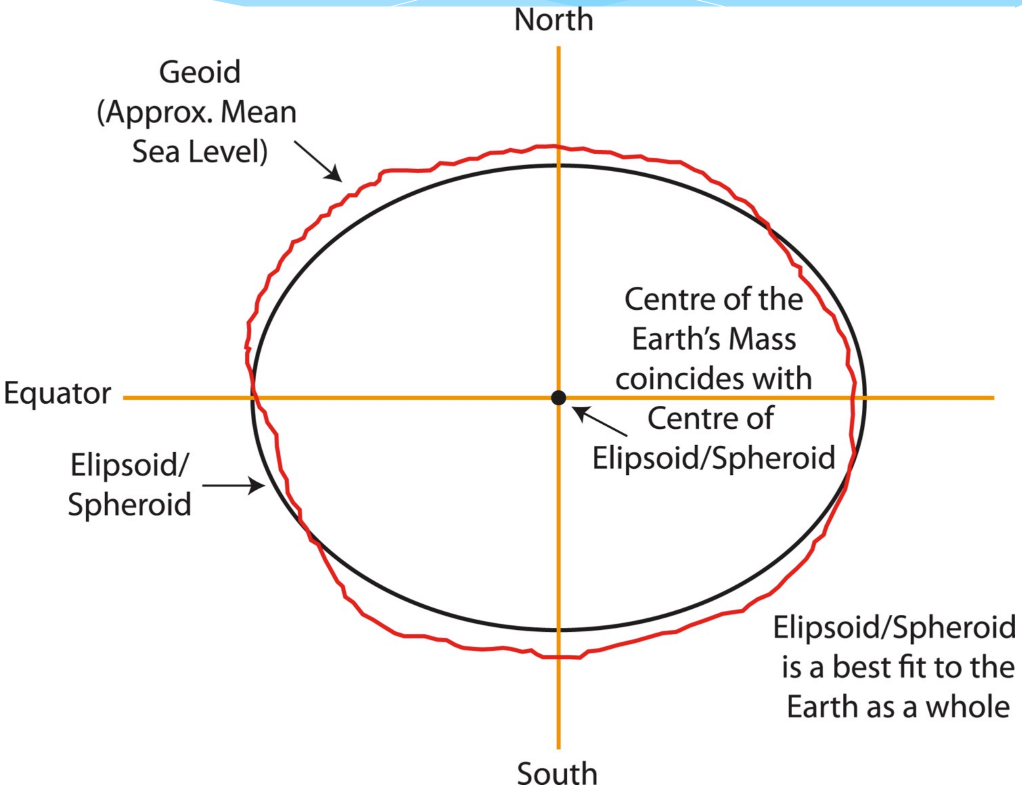
Height of the satellite: ~1340 km

Satellite observation #1: altimetry

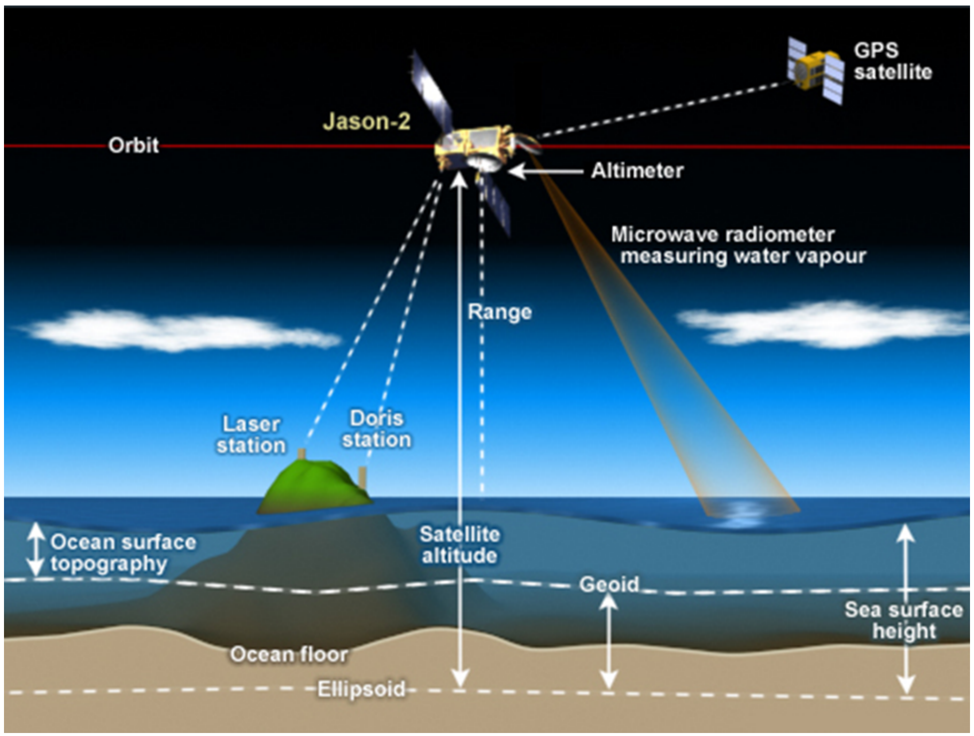
Ellipsoid: theoretical ellipsoidal surface matching approximately the shape of the Earth at sea level.

Geoid: equipotential surface of the effective gravitational field of the Earth at mean sea level.





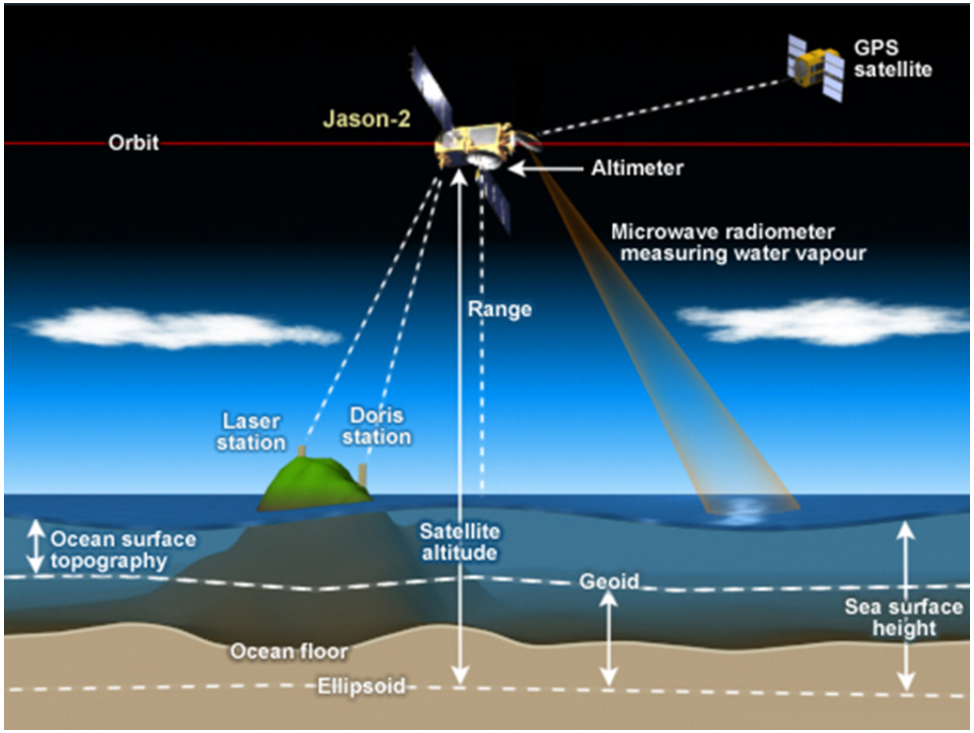
Satellite observation #1: altimetry



The altimeter measures the distance to the surface, R_{alt}, and its own altitude, H_{alt} (ref. ellipsoid). From them we get the sea surface height (SSH):

$$SSH = H_{alt} - R_{alt}$$

Satellite observation #1: altimetry

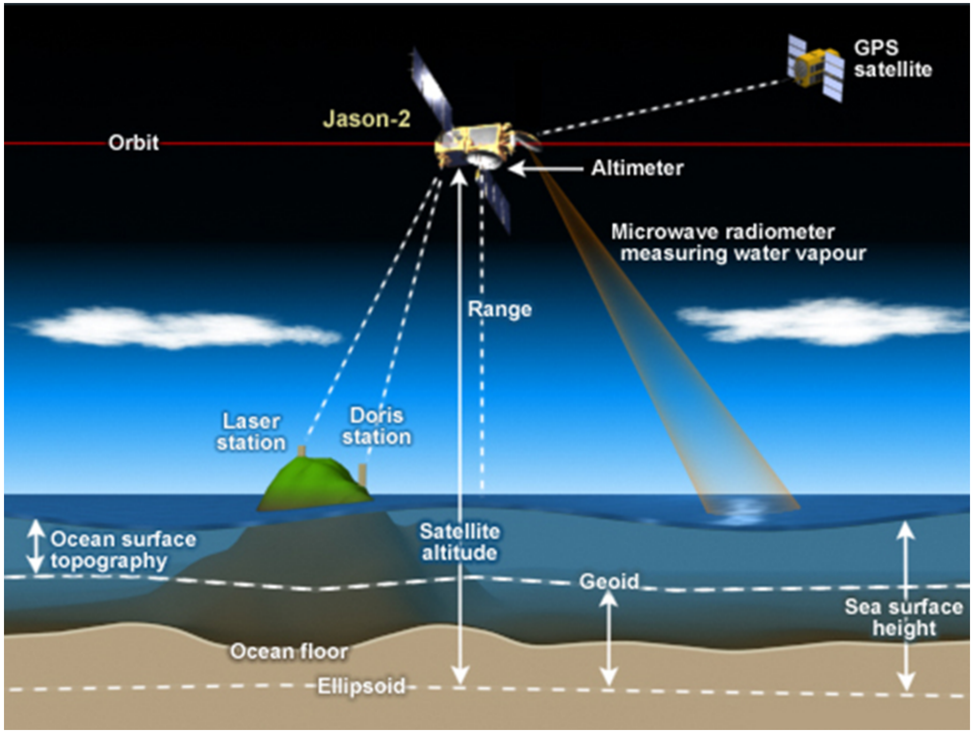


$SSH = H_{alt} - R_{alt}$

The sea surface height (SSH) gathers contributions from gravity (geoid) and ocean surface topography (tides, atmospheric pressure, and ocean dynamics):

$SSH = h_{geoid} + h_{tide} + h_{atm} + h_{dyn}$

Satellite observation #1: altimetry



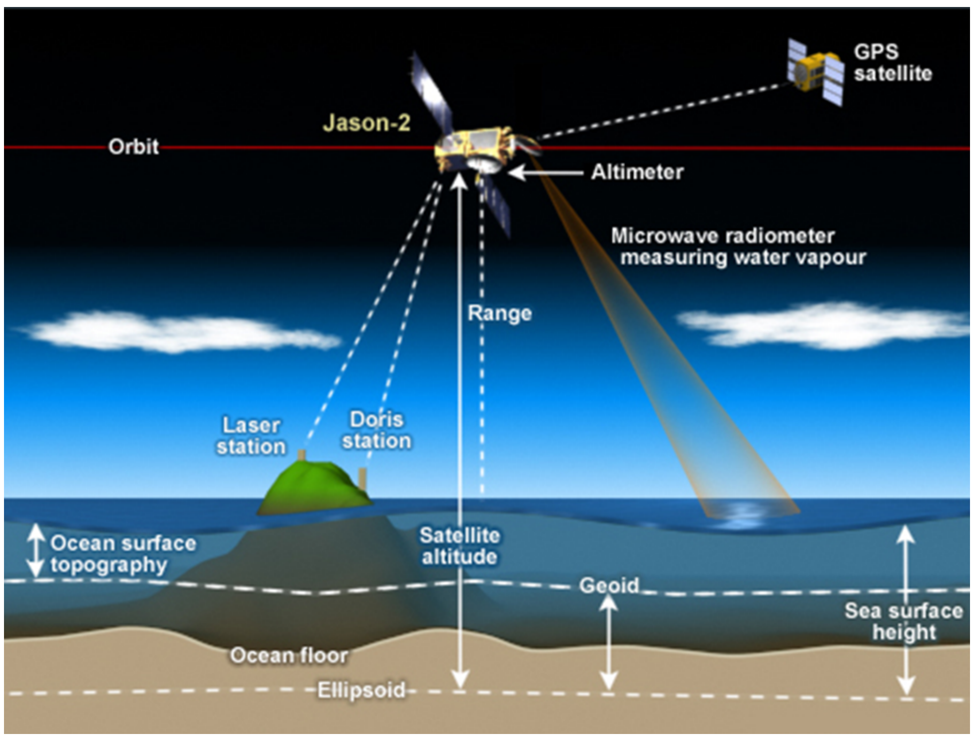
$SSH = h_{geoid} + h_{tide} + h_{atm} + h_{dyn}$

h_{dyn} is the ocean dynamic topography and is due to the motions of the sea. It is the relevant term for studying the ocean circulation.

$h_{dyn=} = H_{alt} - R_{alt} - h_{geoid} - h_{tide} - h_{atm}$

The accuracy of h_{dyn} estimation does not depend only on the altimetric measurement itself.

Satellite observation #1: altimetry



$h_{dyn=}$=H_{alt}-R_{alt}-h_{geoid}-h_{tide}-h_{atm}

Precisions:
H_{alt}: 2 cm
h_{tide}: 2 cm

h_{atm} correction is based on atmospheric models.

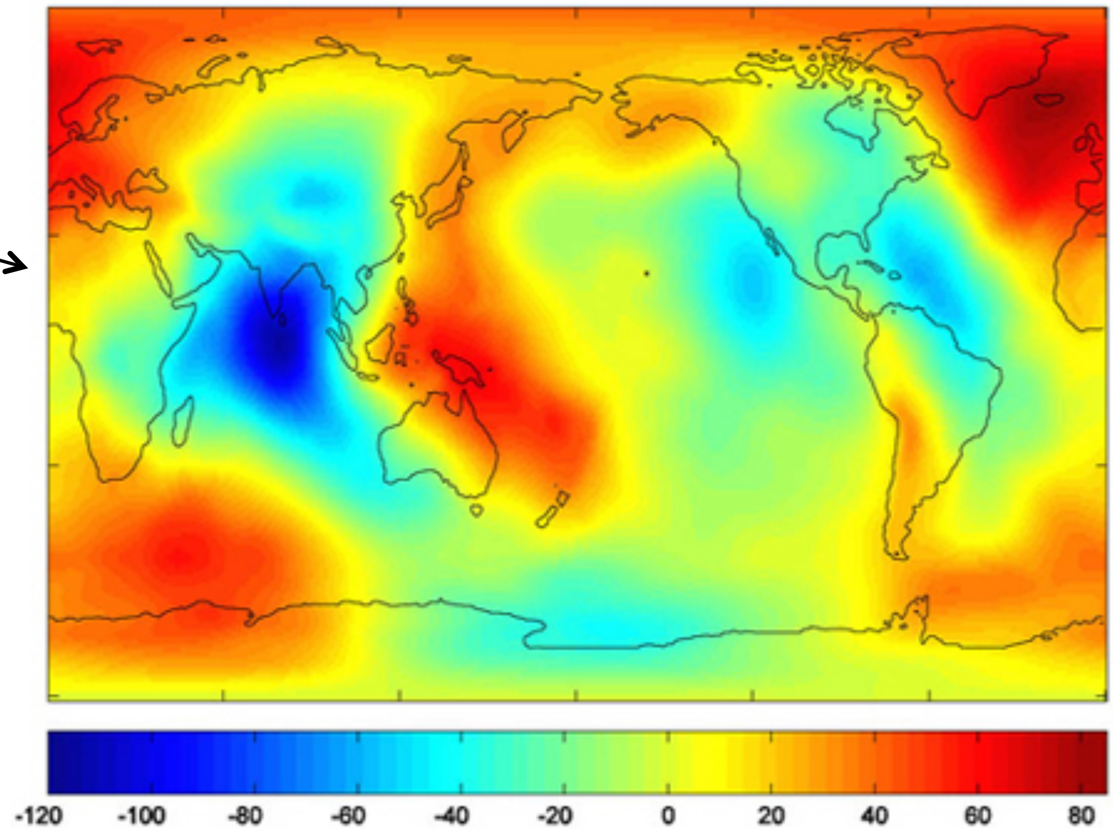
h_{geoid} is the big issue.

Satellite observation #1: altimetry

Recent satellite missions provides a geoid: GOCE, GRACE.

But so far we keep h_{dyn} $+h_{geoid}$ and substract the time mean over many orbit cycles to obtain the sea level anomaly (SLA).

SLA does not contain any information about the mean ocean circulation.



(University of Texas Center for Space Research and NASA)

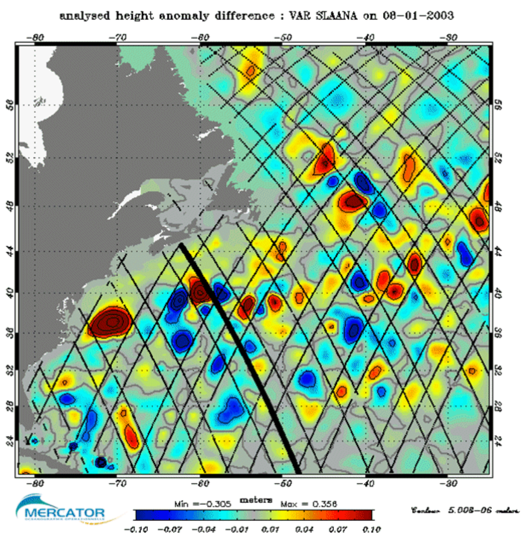
Satellite observation #1: altimetry

Obtaining a "good" SLA products usable in ocean DA systems requires a complex data post-processing, from quality control to calibration…

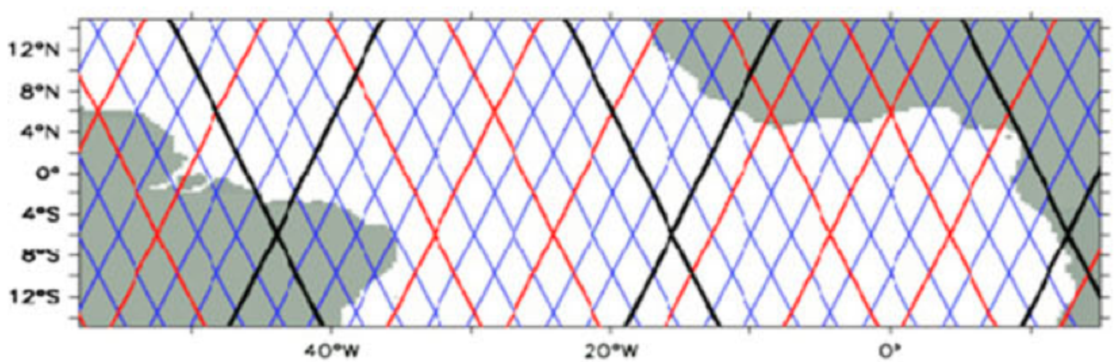
This is performed by the company CLS (Collecte Localisation Satellites), affiliate of CNES and IFREMER, within the project AVISO:

http://www.aviso.altimetry.fr/

Satellite observation #1: altimetry



Orbit of Jason:
Cycle of 10 days.



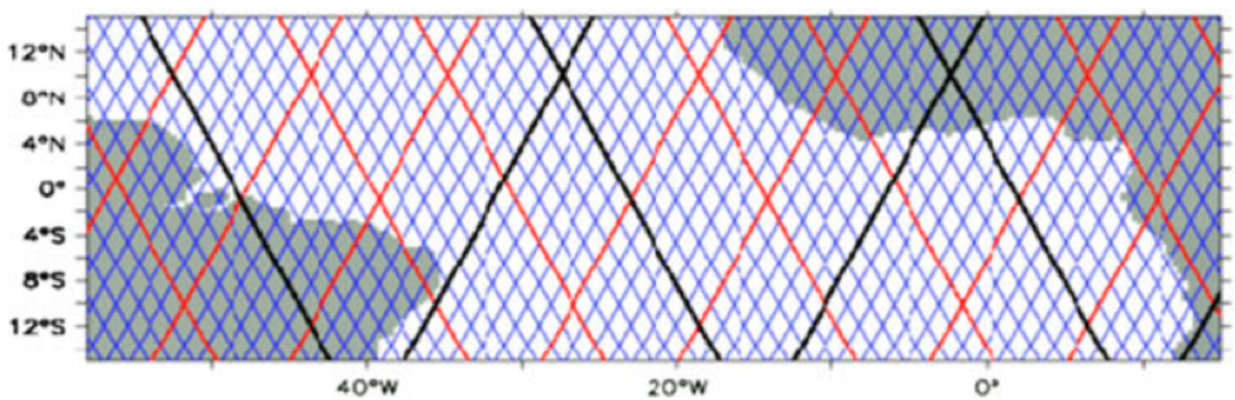
Orbit-1 (Jason)

H=1336km i=66°

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

Satellite observation #1: altimetry

Orbit of GFO:
Cycle of 17 days.



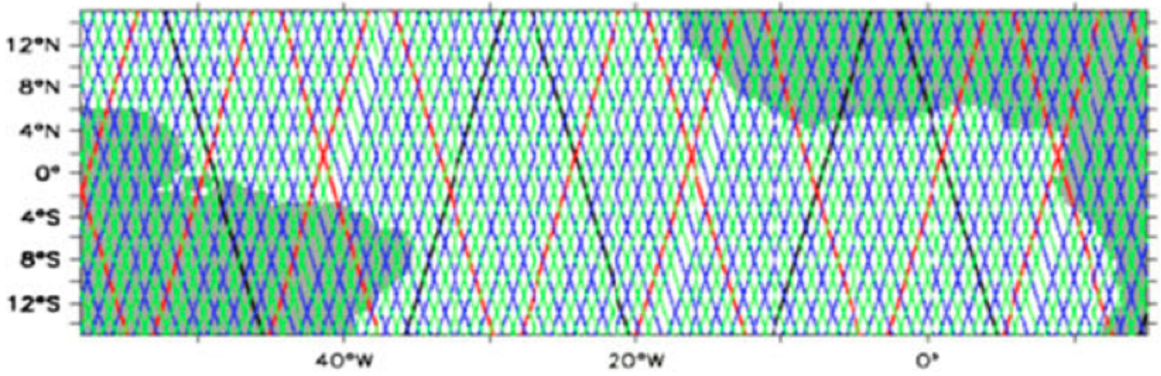
Orbit-2 (Gfo) : H=800km i=108°

H=800km i=108°

(sub-)cycles (days) : **1.0** **2.8** **17.0**

Satellite observation #1: altimetry

Orbit of Envisat and Saral:
Cycle of 35 days



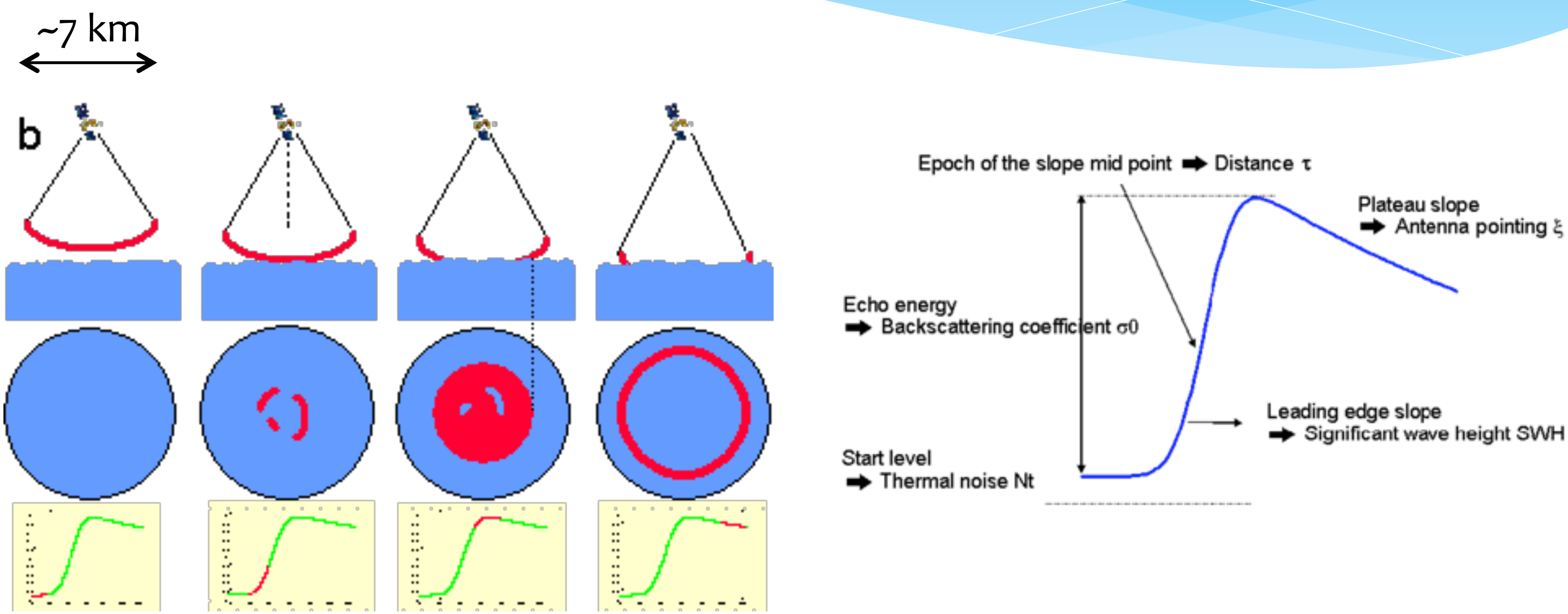
Orbit-3 (Envisat, Saral

H=782km i=98°

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

Observations

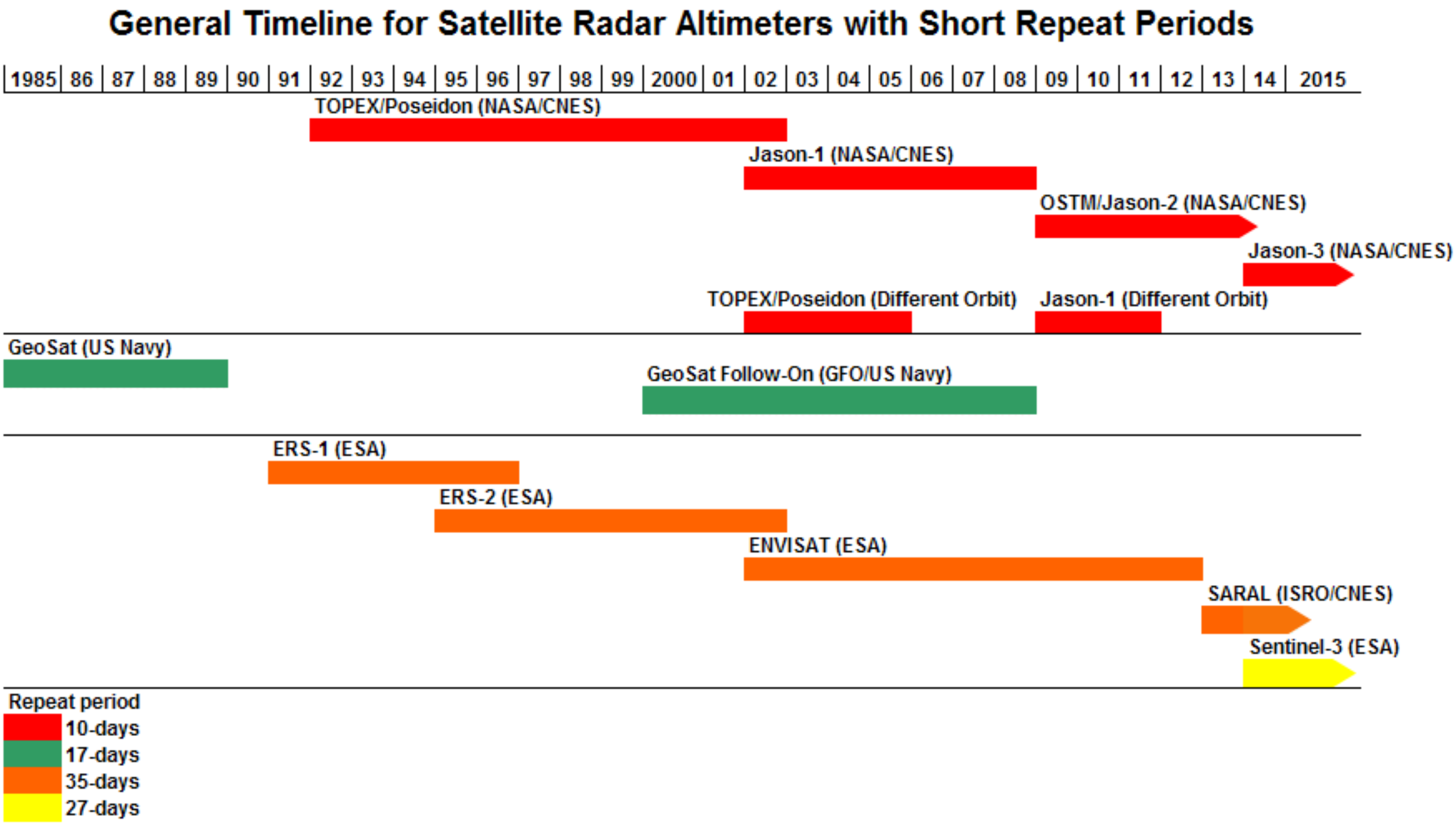
Satellite observation #1: altimetry



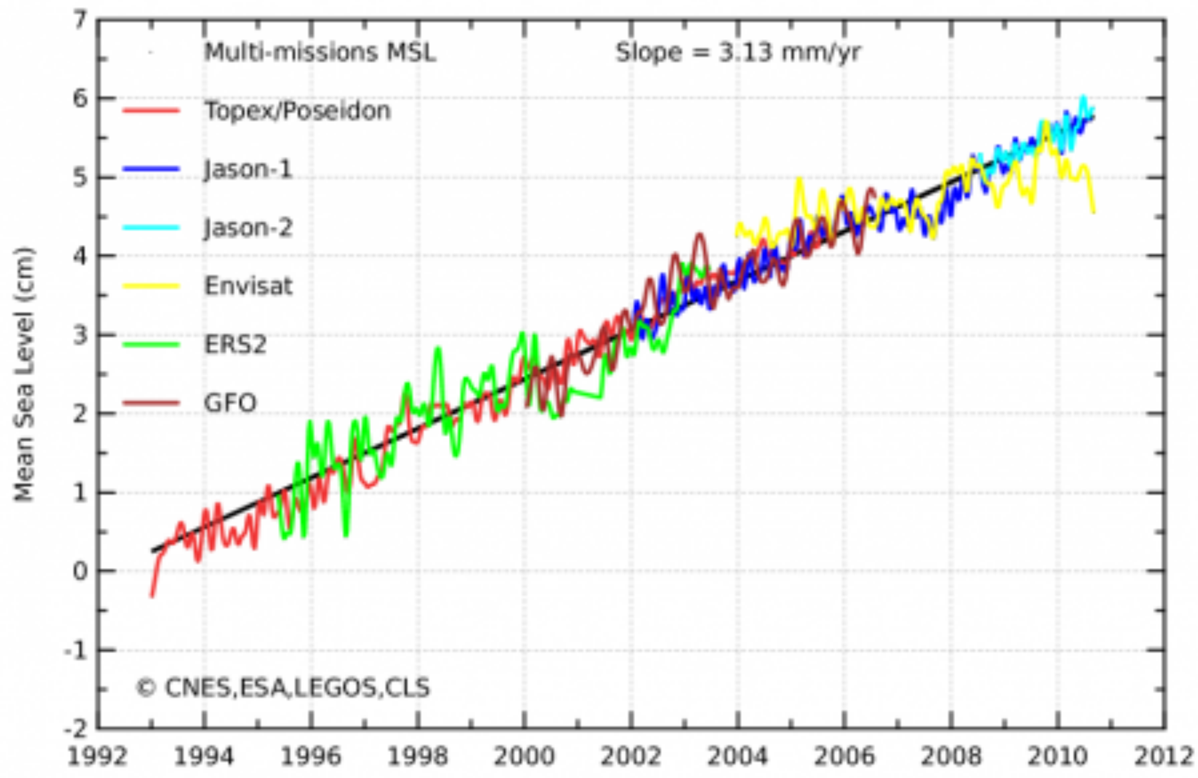
Radar altimetry provides information about mesoscale ocean topography (50-100 km) and waves.

Observations

Satellite observation #1: altimetry



Satellite observation #1: altimetry



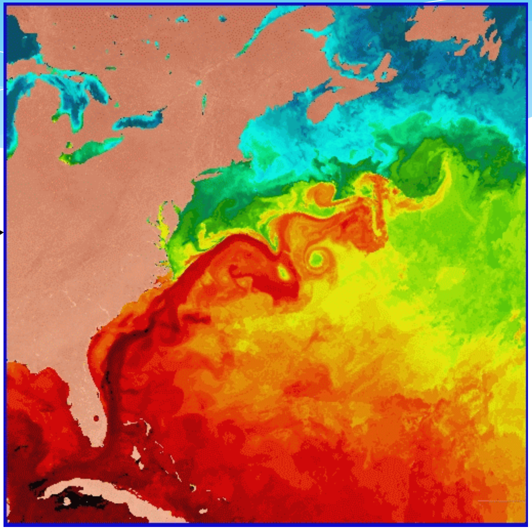
The continuity of satellite altimeters is essential for monitoring the mean sea level.

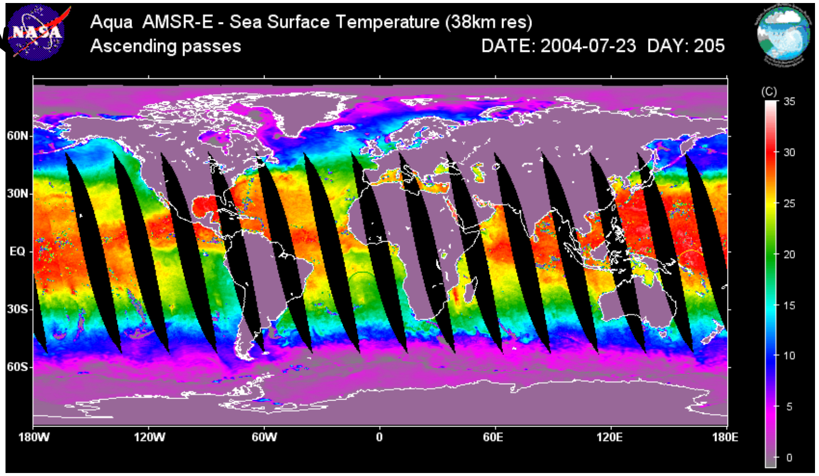
Satellite observation #2: SST

- 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.





Satellite observation #2: SST

IR sensors records the radiance detected at the top of the atmosphere in various bands, linked to temperature by the Planck equation (black body emission):

$$L(\lambda, T) = \frac{C_1}{\pi\lambda^5[\exp(C_2/\lambda T) - 1]}$$

The spectral radiance is transformed into a brightness temperature after direct calibration of the sensors using on-board black-body targets.

Atmospheric corrections are derived from the combination of the signals in different spectral bands. Calibration is based on in-situ measurements of SST. Alternative approach: explicit simulation of the atmospheric radiative transfer.

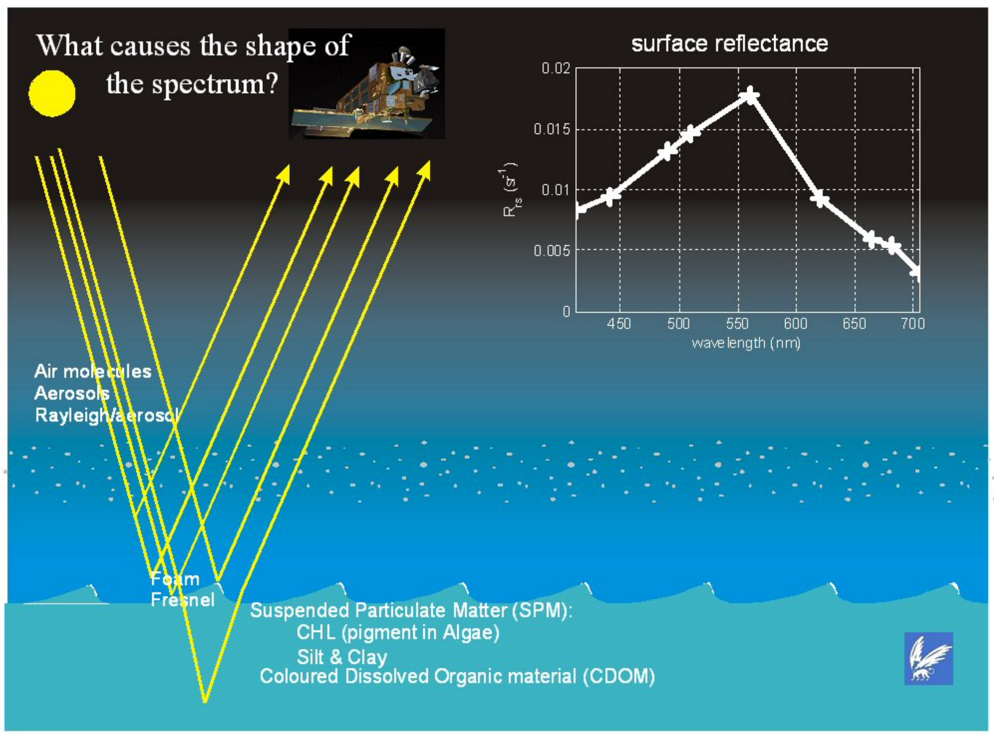
Satellite observation #2: SST

Two issues with satellite SST from the DA viewpoint:

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

Satellite observation #3: Ocean color

Ocean color sensors record reflectances in the solar spectrum.

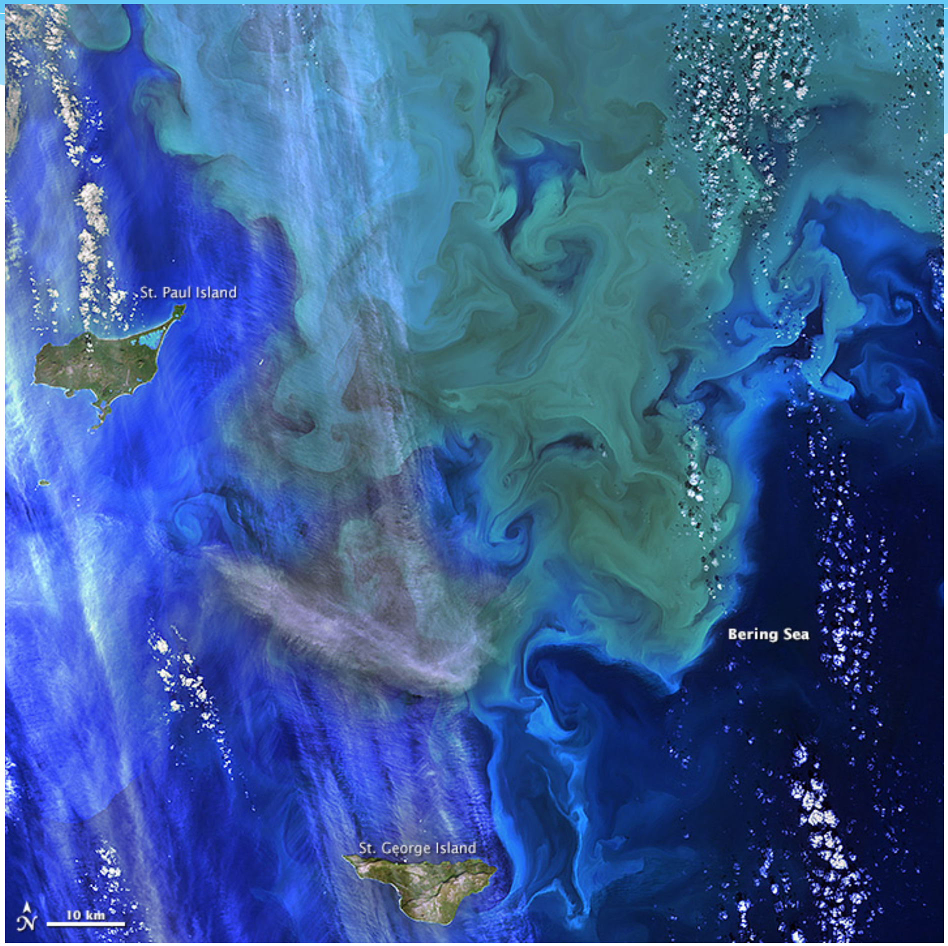


http://www.seos-project.eu/

Satellite observation #3: Ocean color

Ocean color sensors detect chlorophyll.

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



Satellite observation #3: Ocean color

Proof of concept: CZCS (Coastal Zone Color Scanner), 1978-1986.
First operational ocean color products: SeaWIFS (Sea-viewing Wide Field-of-view Sensor), 1997-2010

In addition to the various measurement errors (atmospheric corrections, etc), a significant source of error lies in the algorithm to retrieve chlorophyll concentrations. The accepted error is 30% in general.

Observations: summary

* Quite large diversity of in situ data, but rather sparse;
* A large amount of satellite data, but satellites only see the surface;
* They all contain uncertainties (measurement or representation) that are difficult to estimate.

Ocean DA using Ensemble Kalman filters

* Ensemble Kalman filters
* Localization
* Incremental Analysis Updating (IAU)
* Bogus
* Gaussian anamorphosis
* About the observation error covariance matrix

Ensemble Kalman filters

Kalman filter equations:

Initialization: $\mathbf{x}_0^f$ and $\mathbf{P}_0^f$

Analysis step:

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

Forecast step:

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

Ensemble Kalman filters

Kalman filter equations:

Initialization: $\mathbf{x}_0^f$ and $\mathbf{P}_0^f$

Analysis step:

Too big to store

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

Often too big to invert

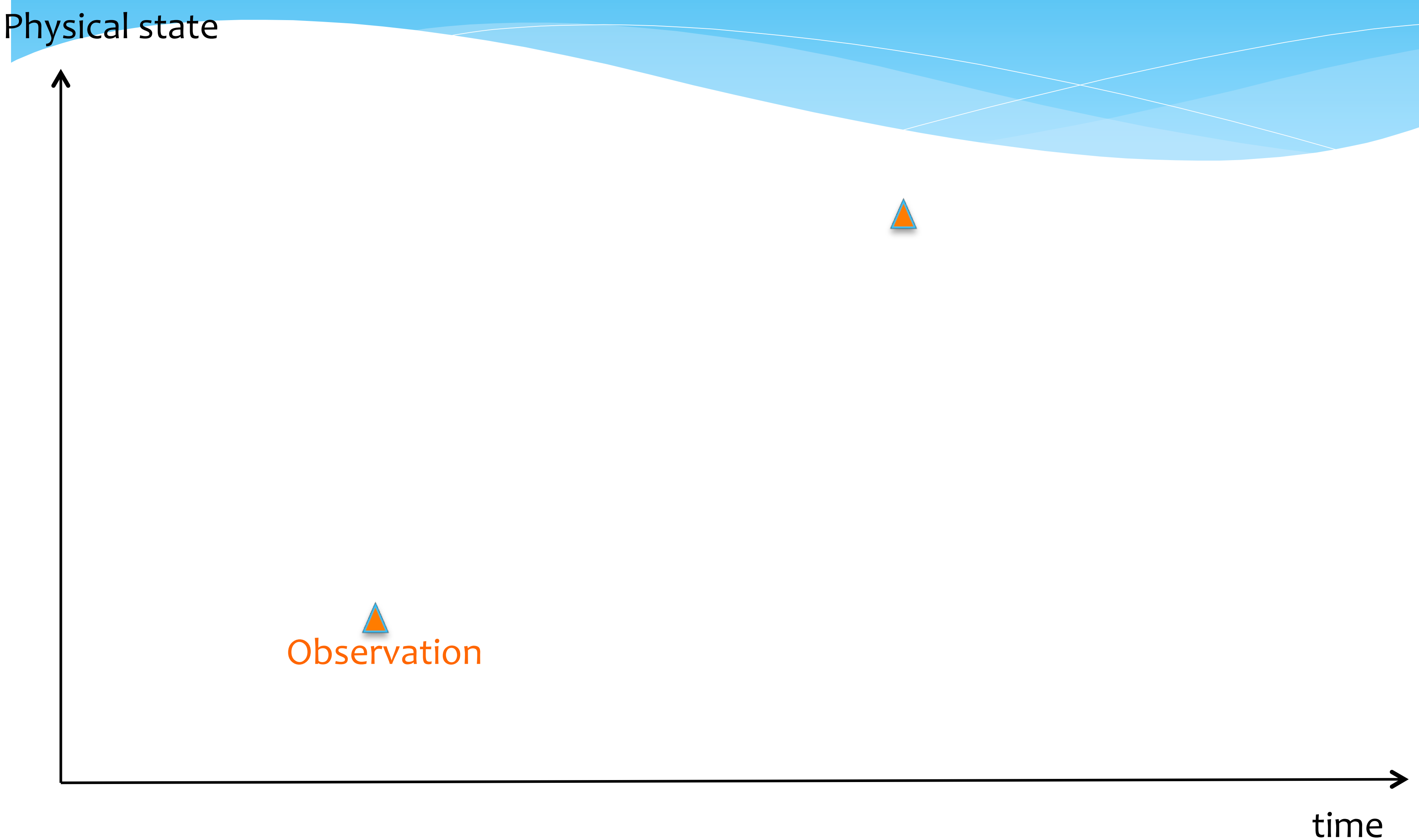
Forecast step:

Often nonlinear in practice

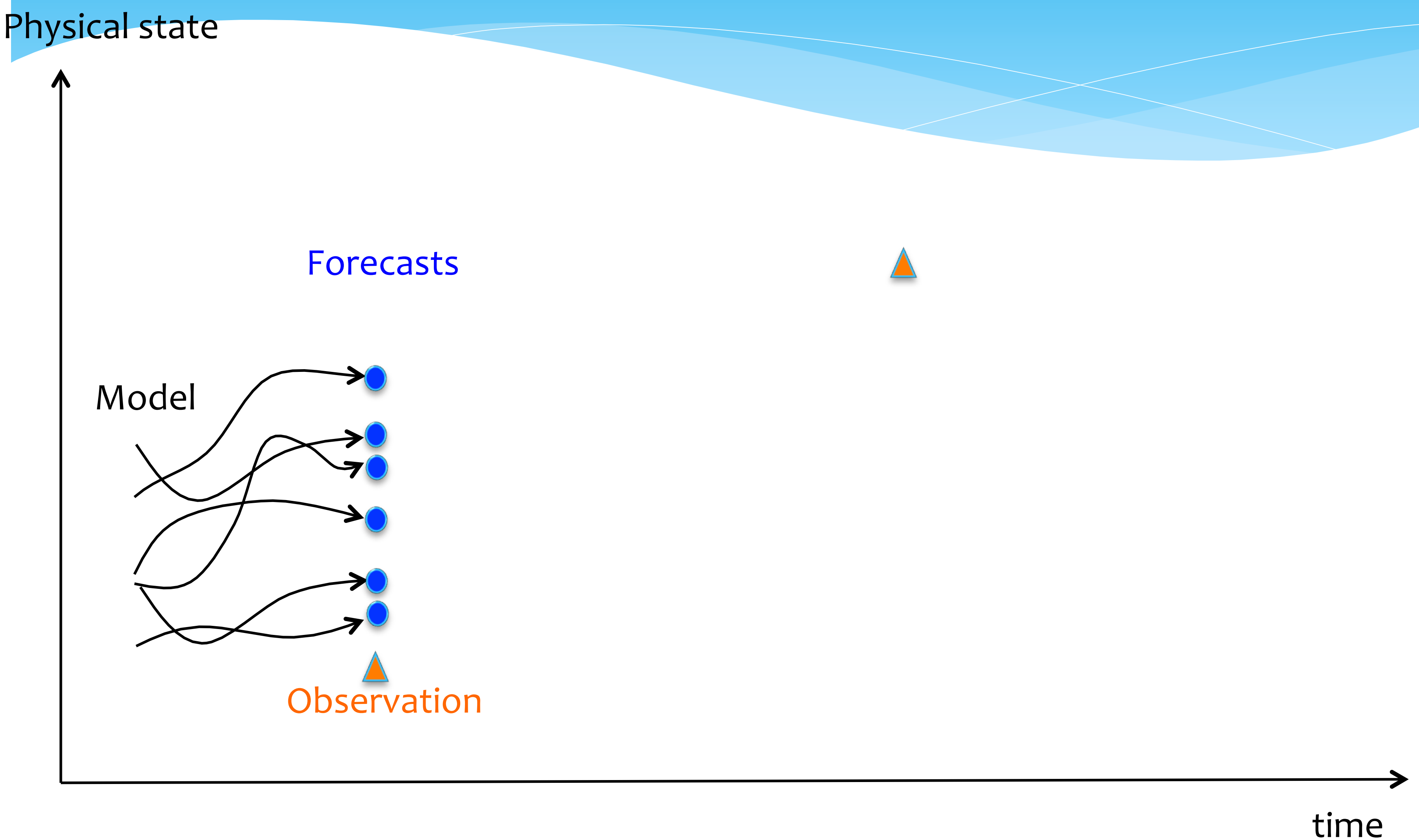
$$
\begin{aligned}
\mathbf{x}_{k+1}^f &= \mathbf{M}_{k,k+1}\mathbf{x}_k^a, \\
\mathbf{P}_{k+1}^f &= \mathbf{M}_{k,k+1}\mathbf{P}_k^a\mathbf{M}_{k,k+1}^T + \mathbf{Q}_k.
\end{aligned}
$$

Rarely that simple, and unknown

Ensemble Kalman filters

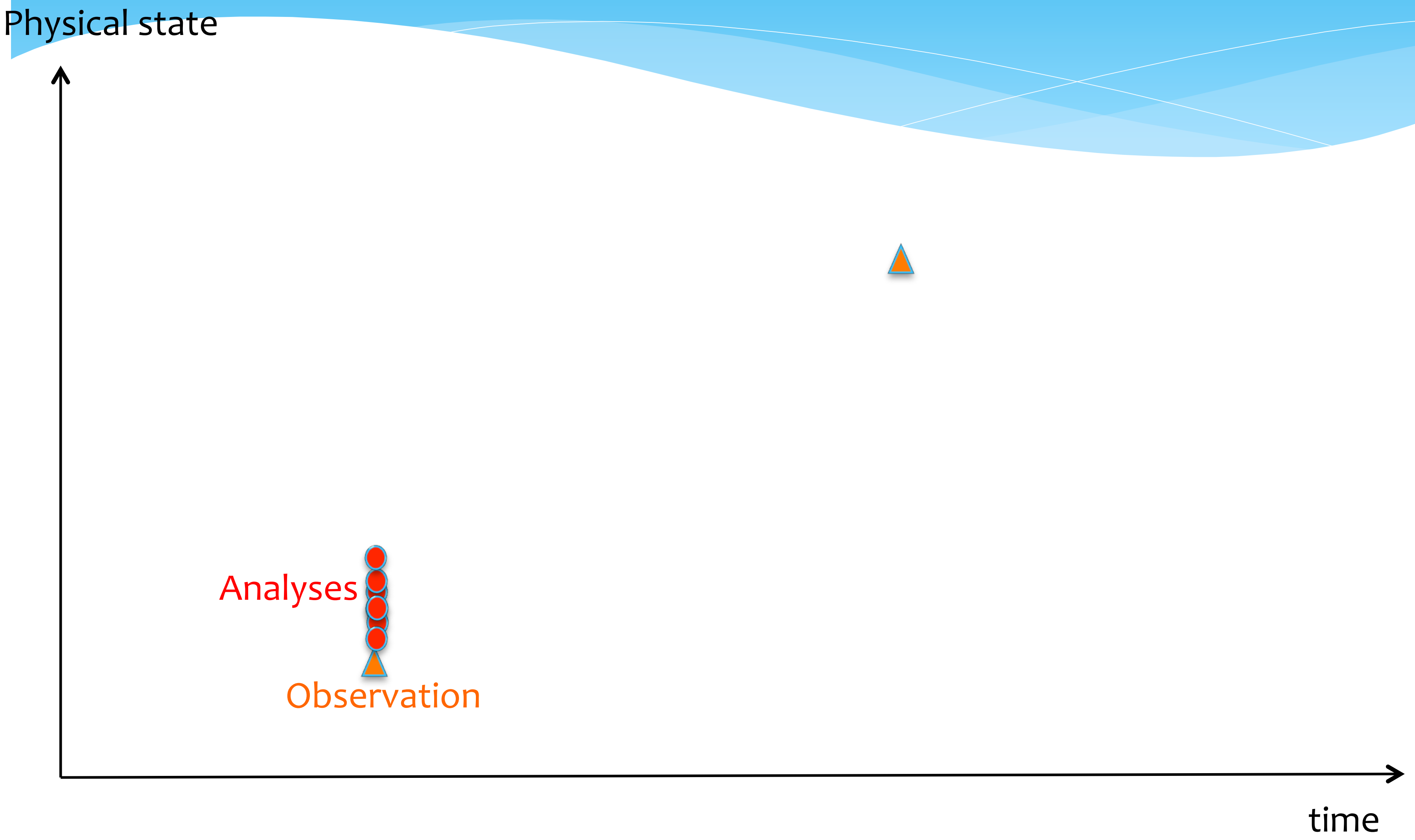


Ensemble Kalman filters

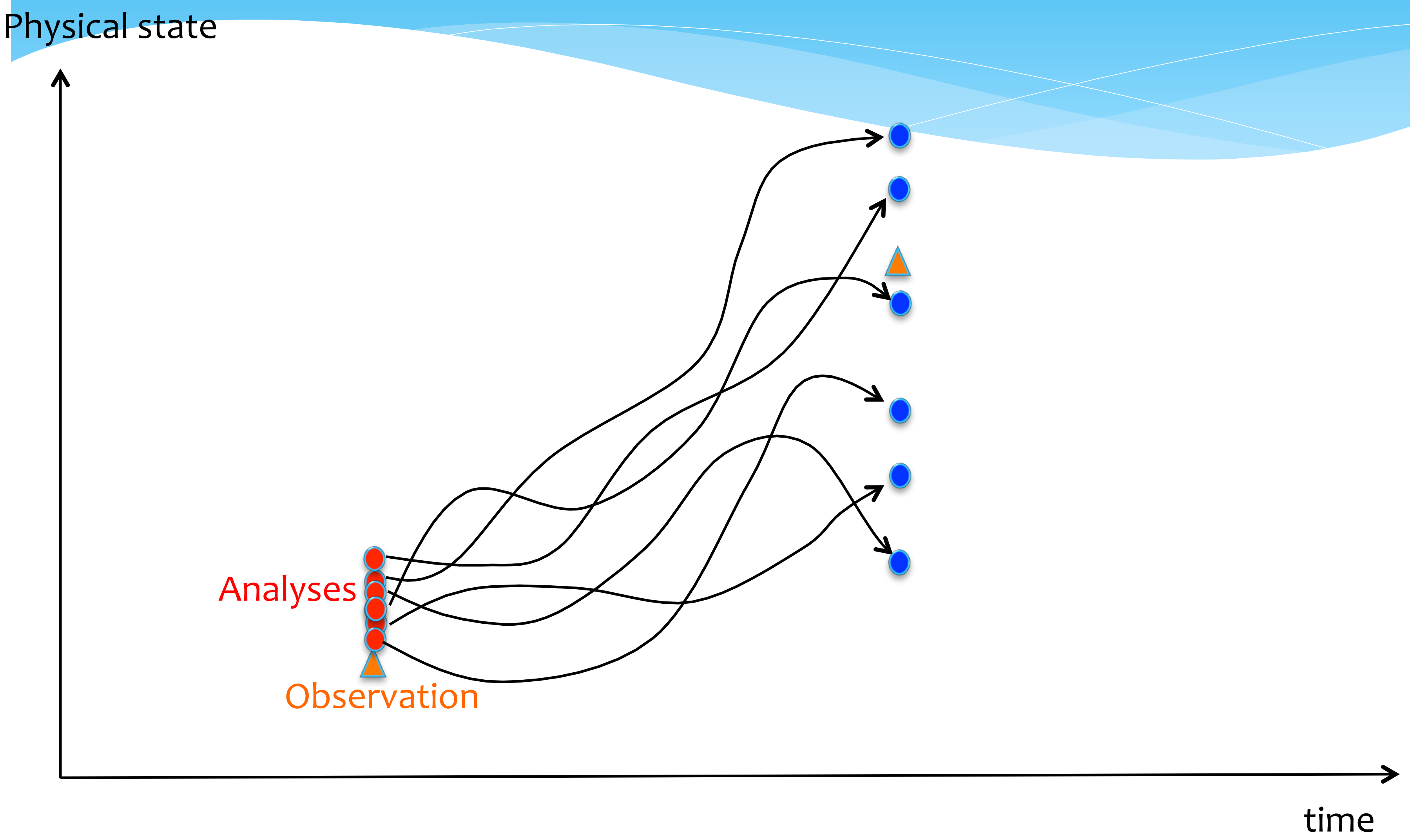


Ocean DA using EnKFs

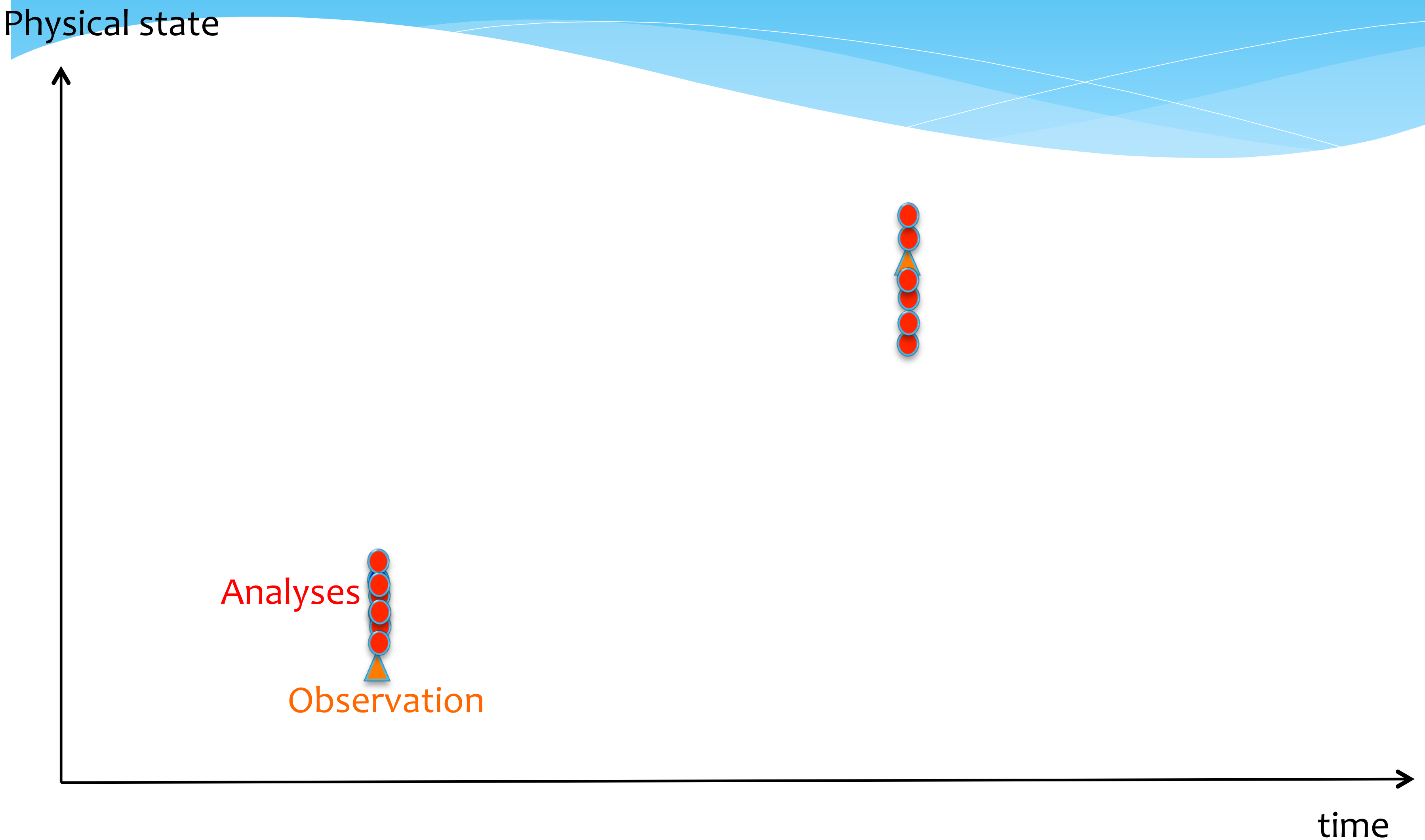
Ensemble Kalman filters



Ensemble Kalman filters

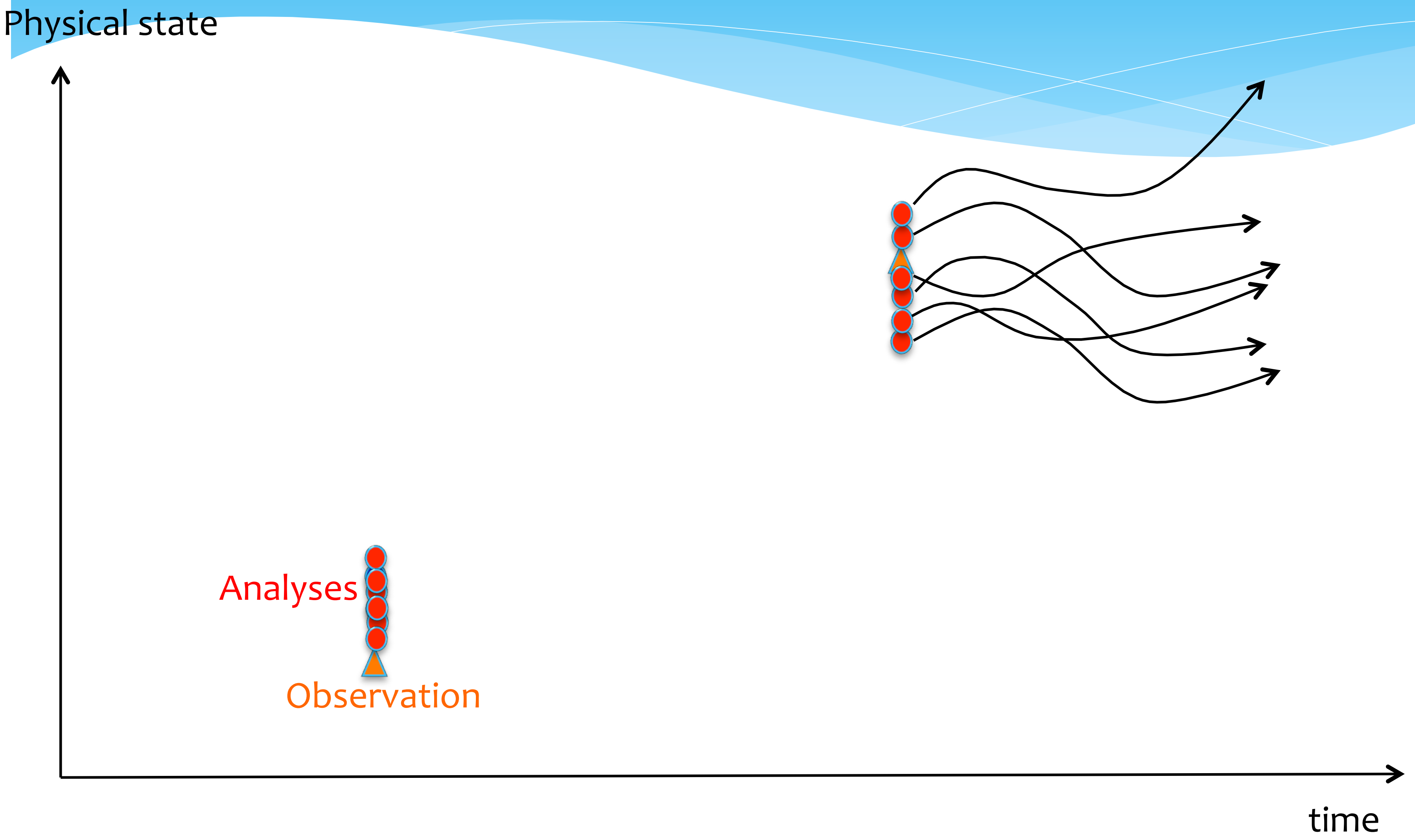


Ensemble Kalman filters



Ocean DA using EnKFs

Ensemble Kalman filters

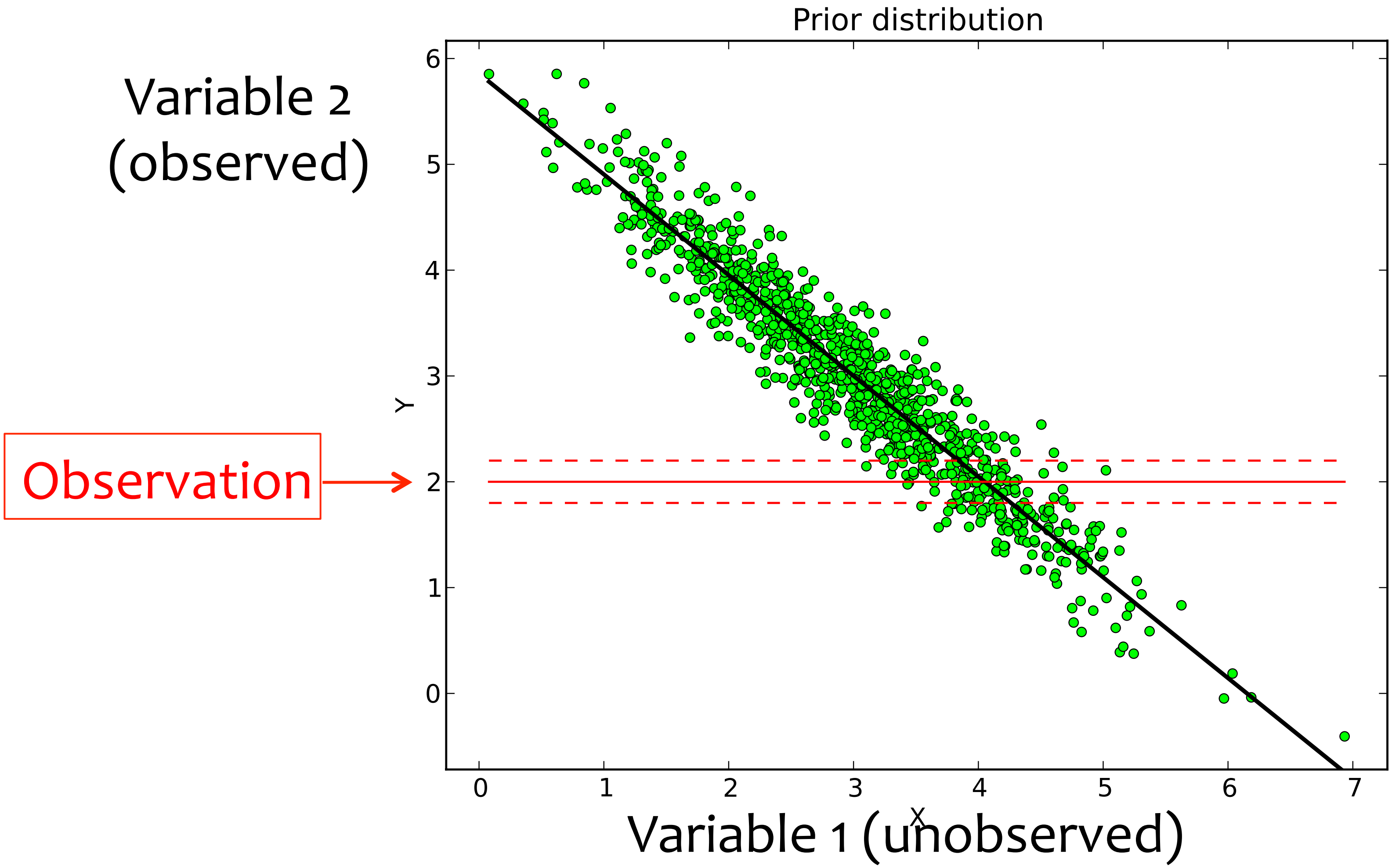


Ensemble Kalman filters

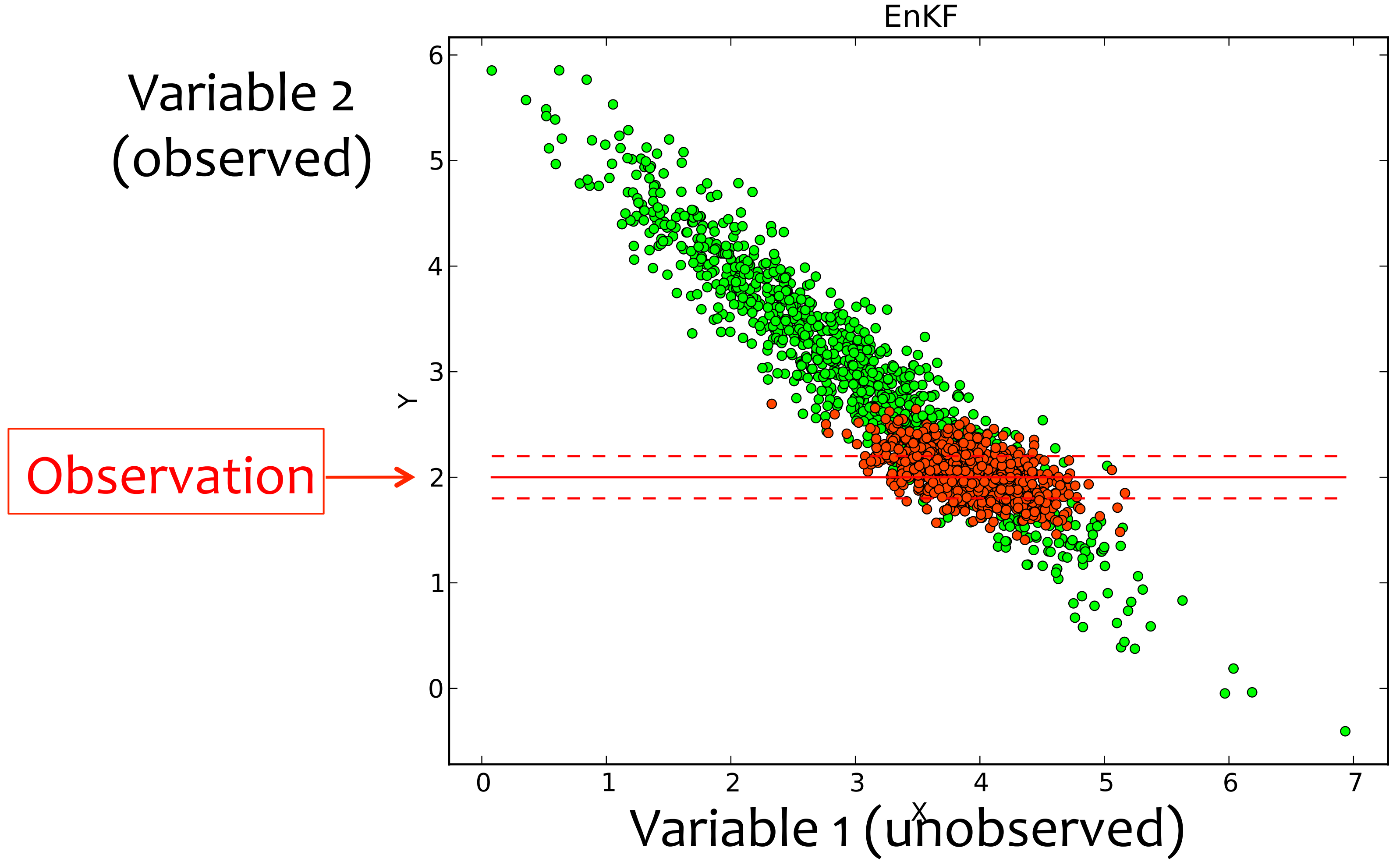
* In the forecast step, each member is advanced with the numerical model:

$$\mathbf{x}^f_{k+1,i} = M_{k,k+1}(\mathbf{x}^a_{k,i}) + \eta_{k,i}$$

Ensemble Kalman filters



Ensemble Kalman filters



Ensemble Kalman filters

* 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

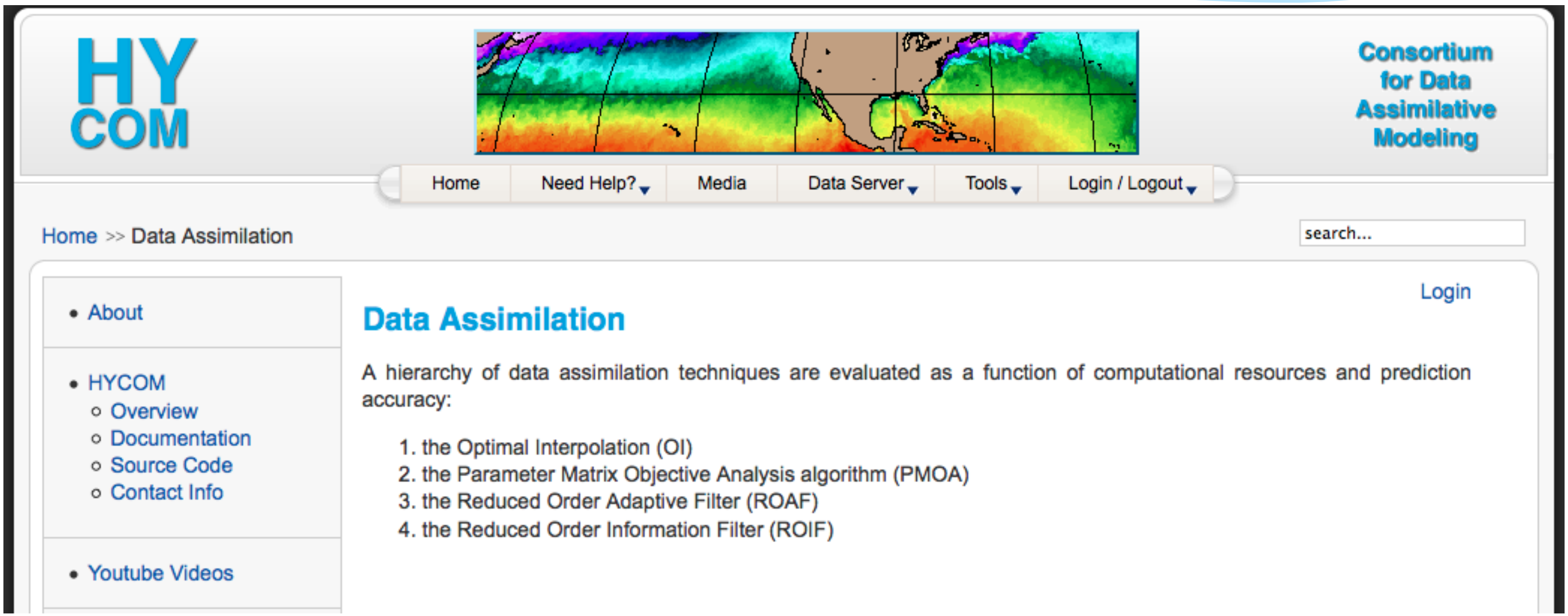
Ensemble Kalman filters

Deliverable 3.1

Contents

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

Ensemble Kalman filters



http://hycom.org/

Ensemble Kalman filters

A simple view

* RRSQRT filters
  * Forecast of 1 (mean) state, and error modes
  * Appropriate to a “fixed basis” approximation
* Stochastic EnKF
  * Correction of each state with perturbed observations
* Deterministic EnKFs
  * Correction of mean and anomalies without perturbing observations

Ensemble Kalman filters

* Ocean DA: $O(10^6 - 10^8)$ variables, $O(10^3 - 10^5)$ 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 Kalman filters

* Ensemble OI = Reduced Rank Square Root filter with a fixed error basis:
  * Only a mean state is propagated with the model;
  * The error modes are the same at any analysis step.
* - - - : no estimation of uncertainties;
* +++: computationally affordable, robust (no collapse), more "physically-based" than historical OI with analytical covariance functions.

Localization

* Localization aims at delimiting in space the impact 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;

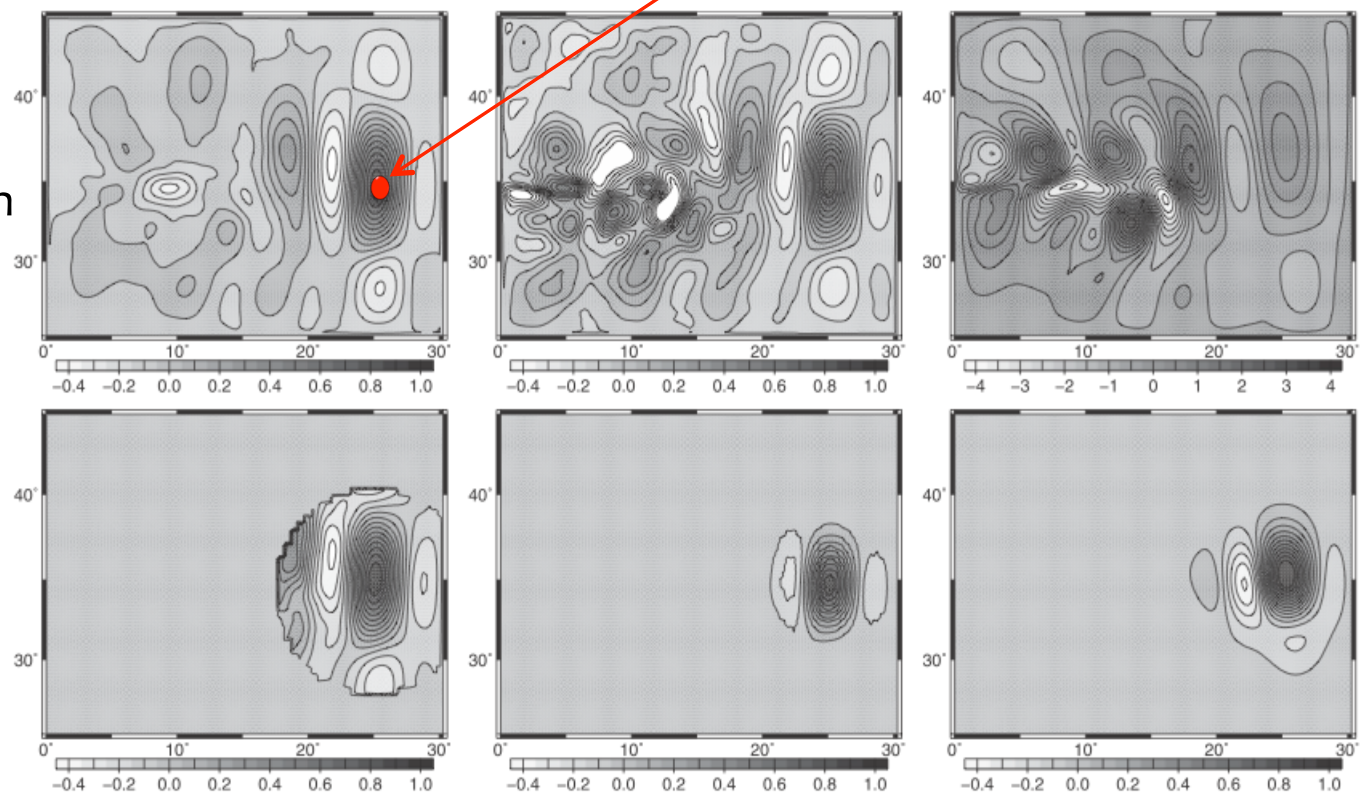
Localization

Increments in SSH due to an observation here

m=5000; no rank reduction | m=200; no rank reduction | m=5000; rank reduction r=20

Without localization

With localization



m=200; no rank reduction
Awkward localization

m=200; no rank reduction

m=5000; rank reduction r=20

(Brankart et al, 2011)

Localization

* Localization aims at delimiting in space the impact 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.

Localization

* Why increasing the rank of the covariance matrix?
* Remember that in the ETKF, the correction on the mean is a linear combination of the anomalies (see Marc Bocquet's course, Eq. 5.34):

$$\mathbf{x}_i^a = \bar{\mathbf{x}}^f + \mathbf{X}^f \gamma_i$$

* There is only m (ensemble size, ~10-100) degrees of freedom to correct a vector of typical size > 10^6 with 10^3-10^5 observations!

Localization

* Localization aims at delimiting in space the impact 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.

Localization

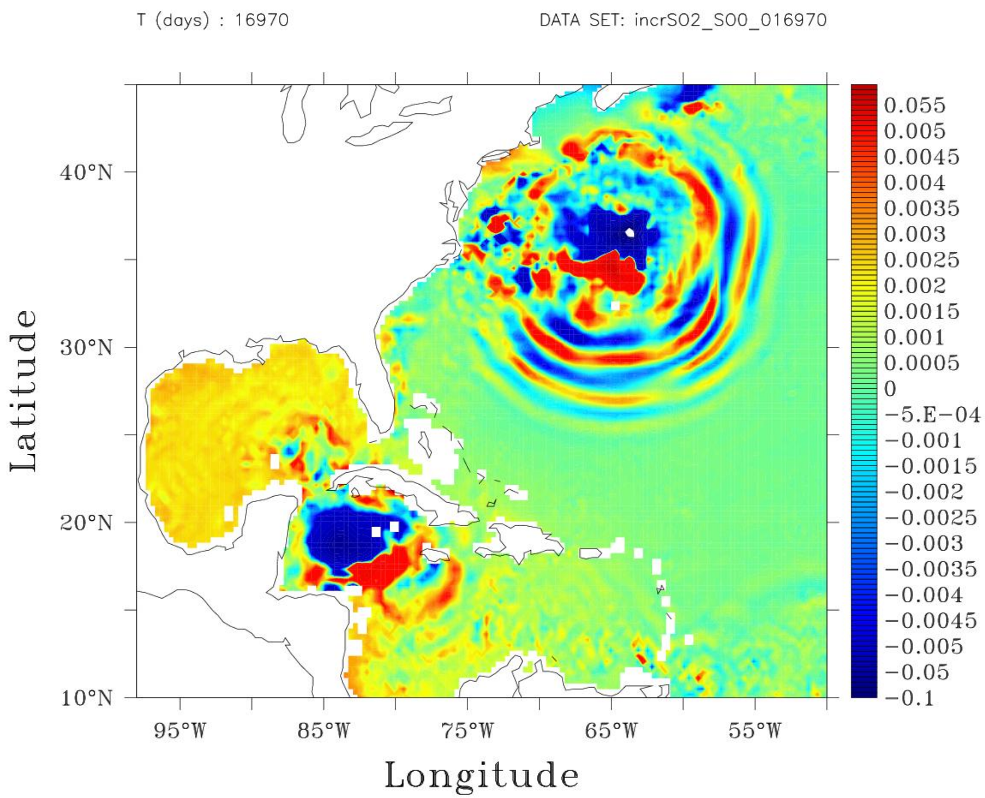
- The Kalman gain can be computed directly if the number of local observations (i.e., the size of *R*) is limited:

$$\mathbf{K}^{*} = \mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}}\left(\mathbf{H}\mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1}$$

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.



(Rozier et al, 2007)

IAU

* 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.

IAU

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).

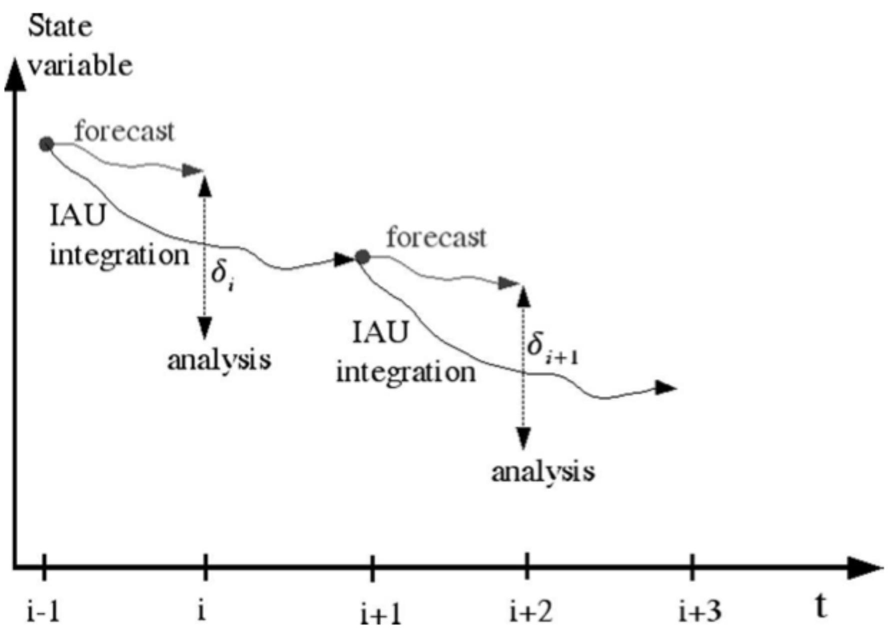


FIG. 1. IAU method from Bloom et al. (1996); δ represents the increment.

IAU

Figure: spatially averaged zonal velocity U in the Gulf Stream zone.
Black: free run
Red: EnOI
Green: EnOI with IAU

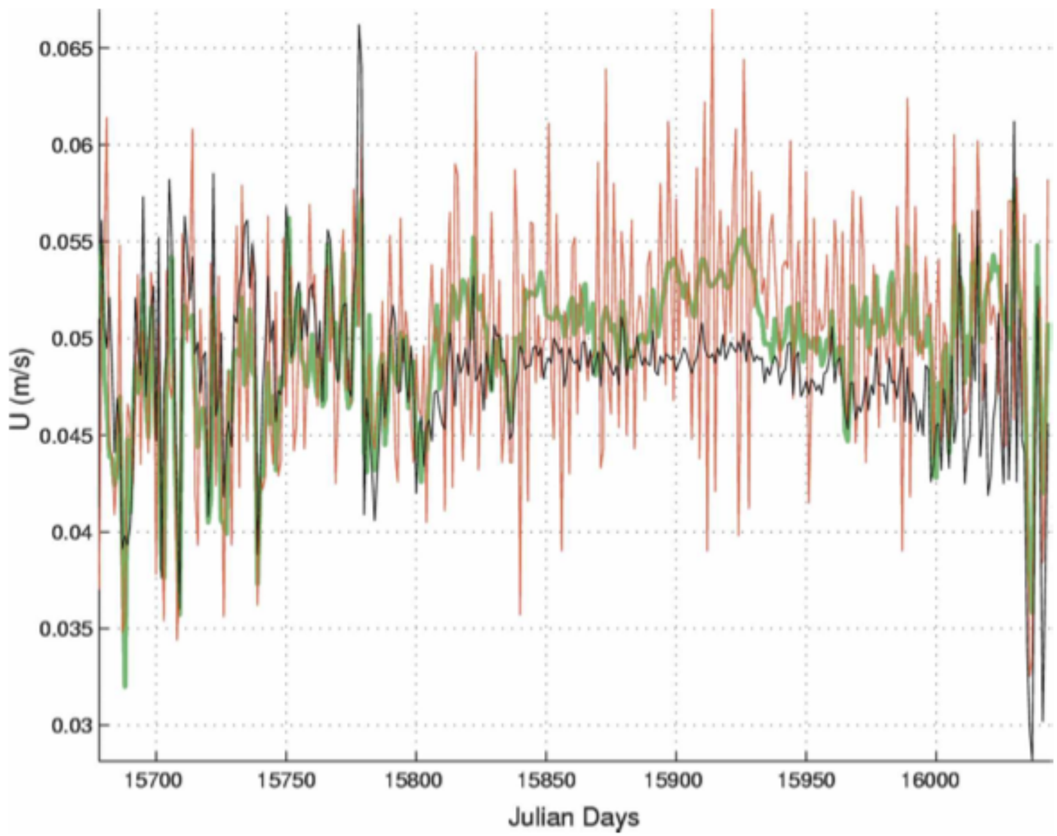


FIG. 12. Same as in Fig. 11, but at a 55-m depth (model depth level 5) from Julian day 15678 (4 Dec 1992) to 16038 (5 Dec 1993): black line represents FREE run, red line represents INT run, and green line represents IAU run.

(Ourmières et al, 2005)

Bogus

* Some quantities must be conserved. Example: mass.

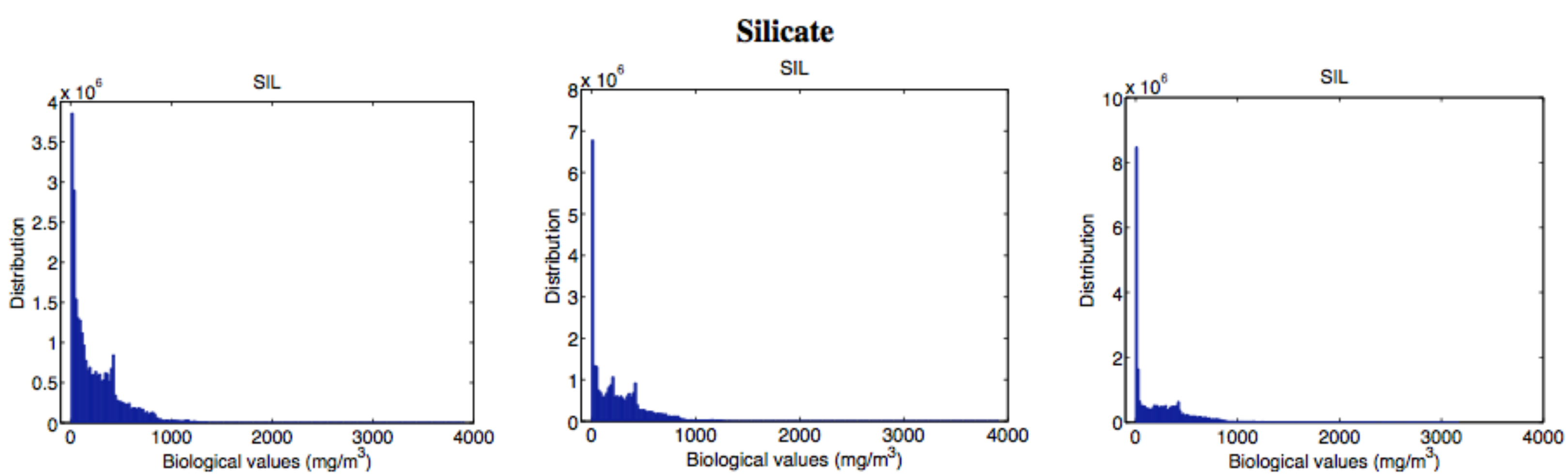
$$\mathrm{div}\ \mathbf{u} = 0$$

* Bogus: a fictitious observation of div **u**, equal to 0.

* Bogus can be used in regions where the assimilation makes things worse…

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)

(Simon et al, 2009)

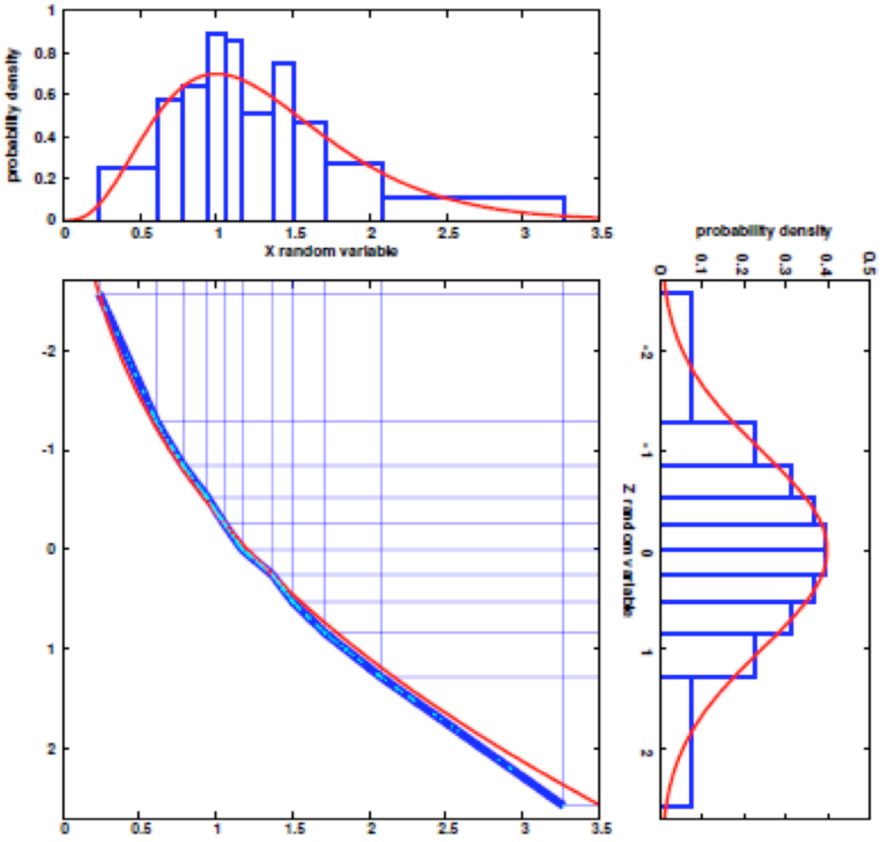
Gaussian anamorphosis

* Sometimes the distribution of some variables does not follow a Gaussian law;
* But the EnKFs are designed for Gaussian variables;
* Gaussian anamorphosis: transformation of a distribution into a Gaussian distribution.

(Bertino et al, 2003)

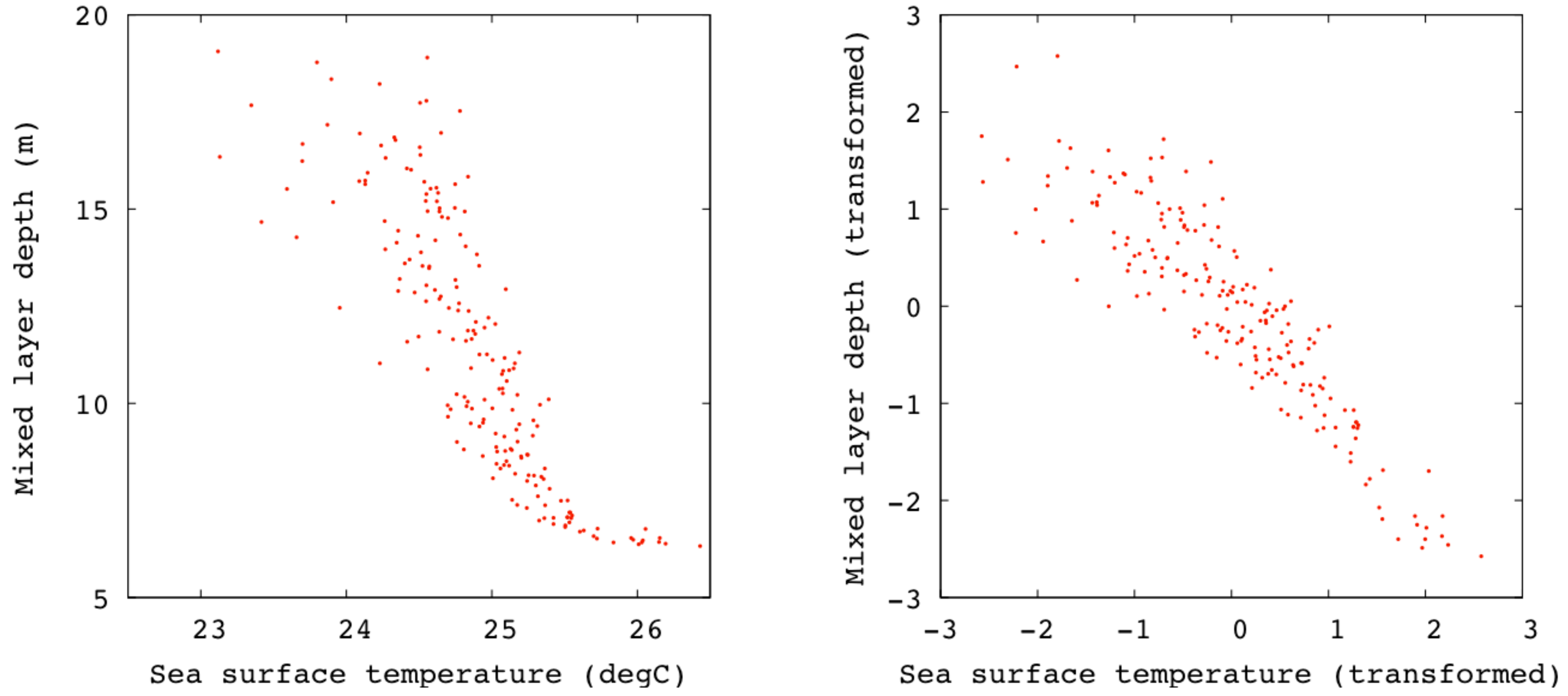
Gaussian anamorphosis

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



(Béal et al, 2010)

Gaussian anamorphosis



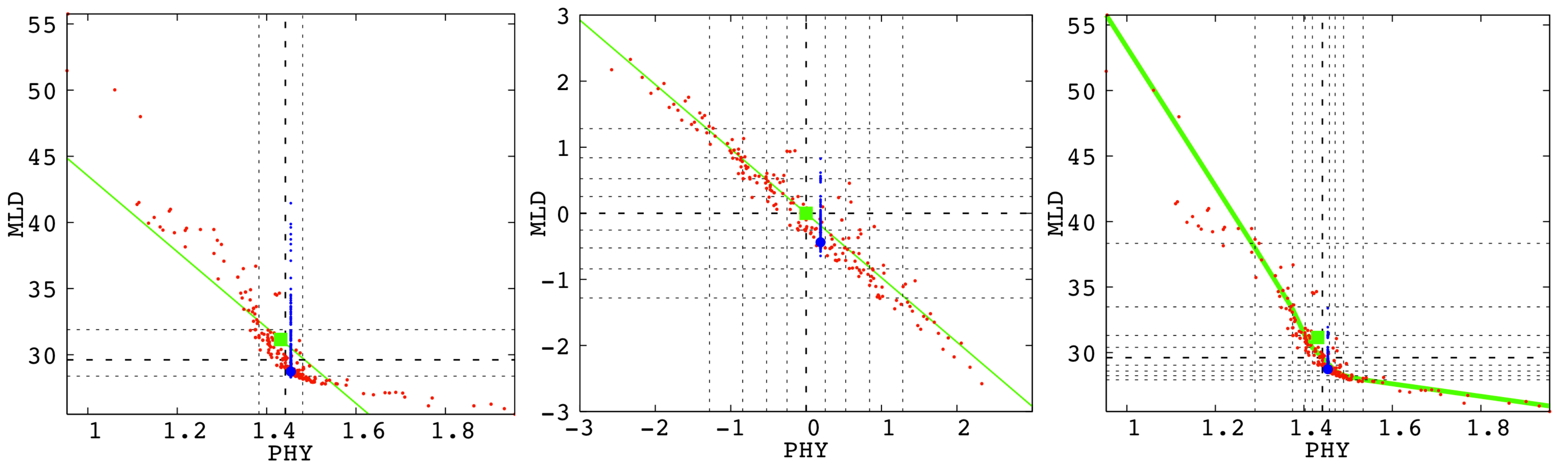
Here, the anamorphosis tends to "Gaussianize" the bivariate distribution.

(Brankart et al, 2012)

Gaussian anamorphosis

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

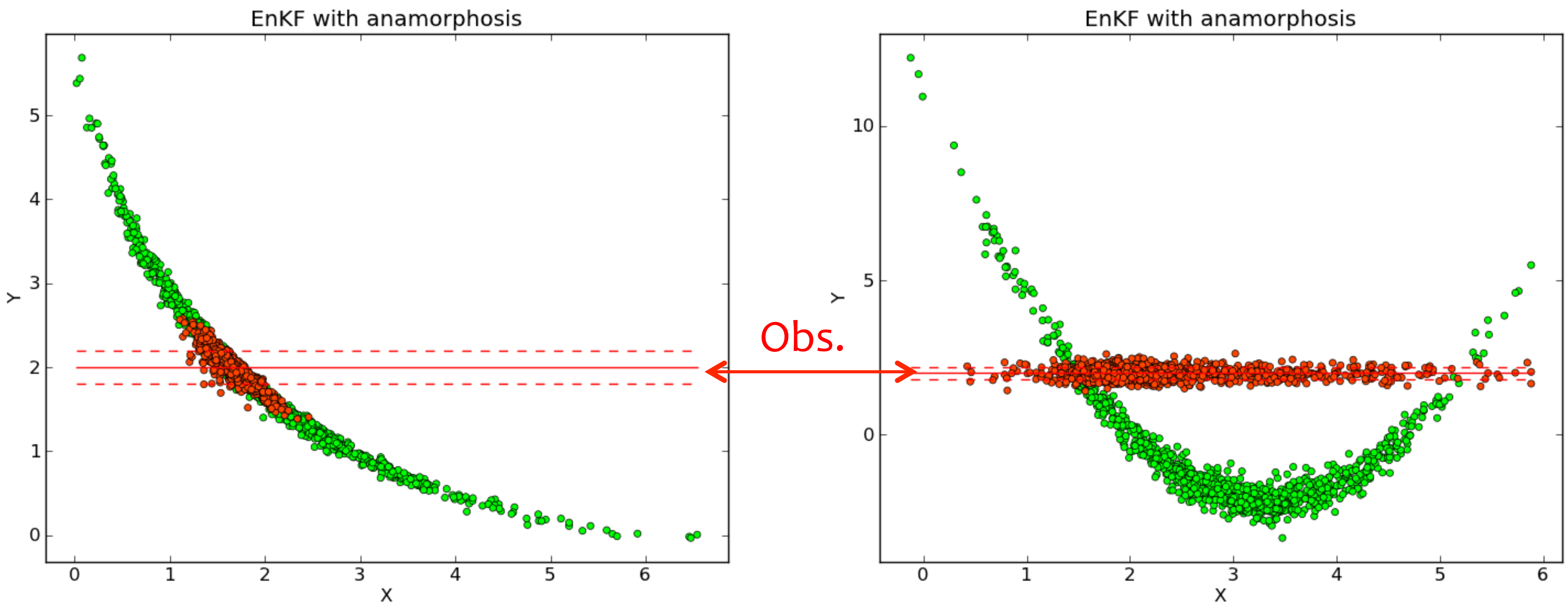
Gaussian anamorphosis



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.

(Béal et al, 2010)

Gaussian anamorphosis



Gaussian anamorphosis works well with weakly non Gaussian variables…

(Metref et al, 2014)

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 $\Gamma = (\mathbf{H}\mathbf{S}^f)^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{S}^f)$

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

About the observation error covariance matrix

* 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.

Ocean DA using variational methods

* Variational methods
* Incremental 4DVar
* Parameterization of the covariance matrix

Variational methods

* Problem posed as the minimization of a cost function to find the best compromise between a prior knowledge x^b and observations y:

$$J(x) = \underbrace{\boxed{\frac{1}{2}\|x - x^b\|_b^2}}_{J_b} + \underbrace{\boxed{\frac{1}{2}\|H(x) - y\|_o^2}}_{J_o}$$

* With respect to a control vector x to choose carefully (very often: initial condition)

Variational methods

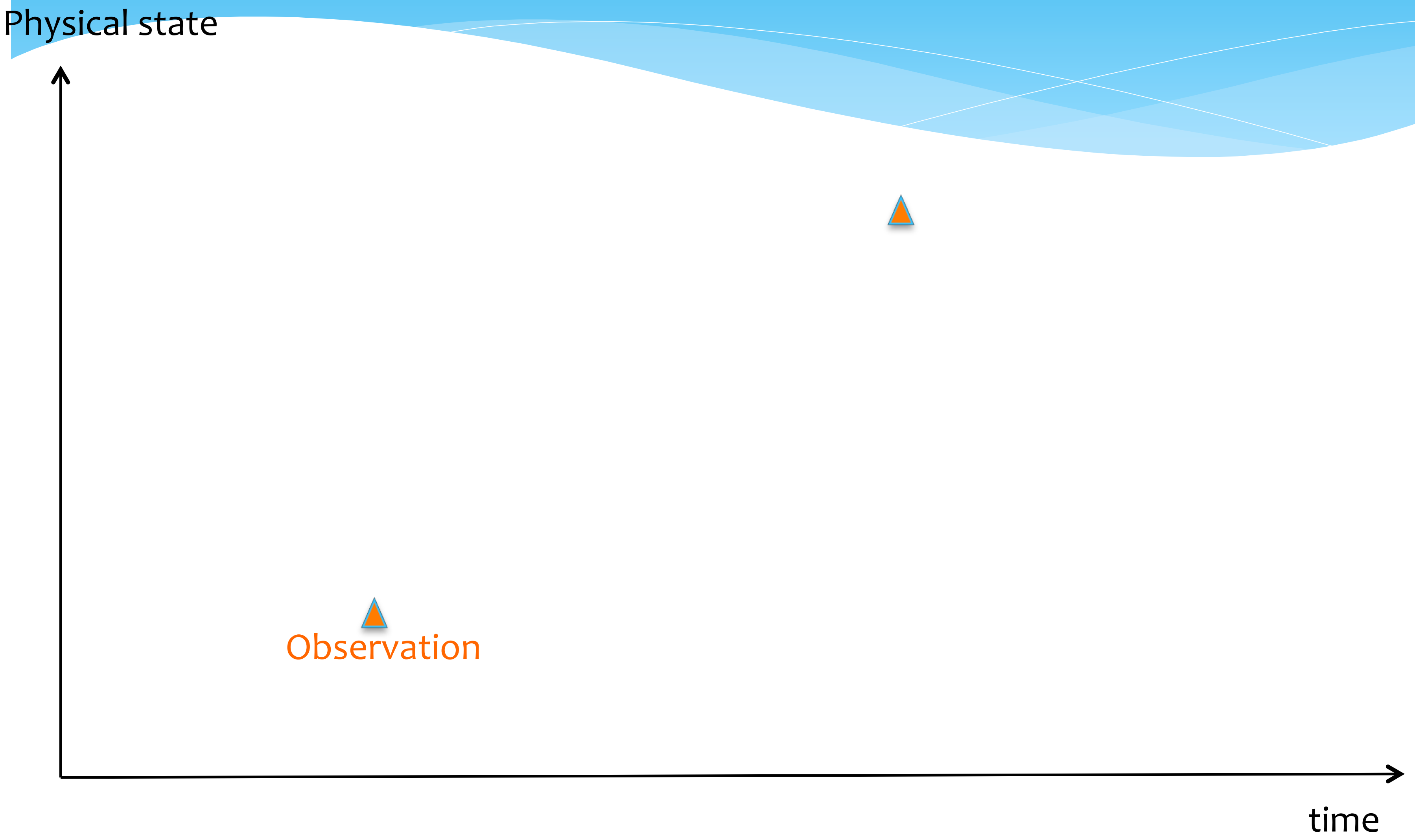
* 3DVar and 4DVar: the cost functions are quadratic.

$$J_{3D}(x_0) = \frac{1}{2}(x_0 - x^b)^T\mathbf{B}^{-1}(x_0 - x^b) + \frac{1}{2}(H(x_0) - y_0)^T\mathbf{R}^{-1}(H(x_0) - y_0)$$

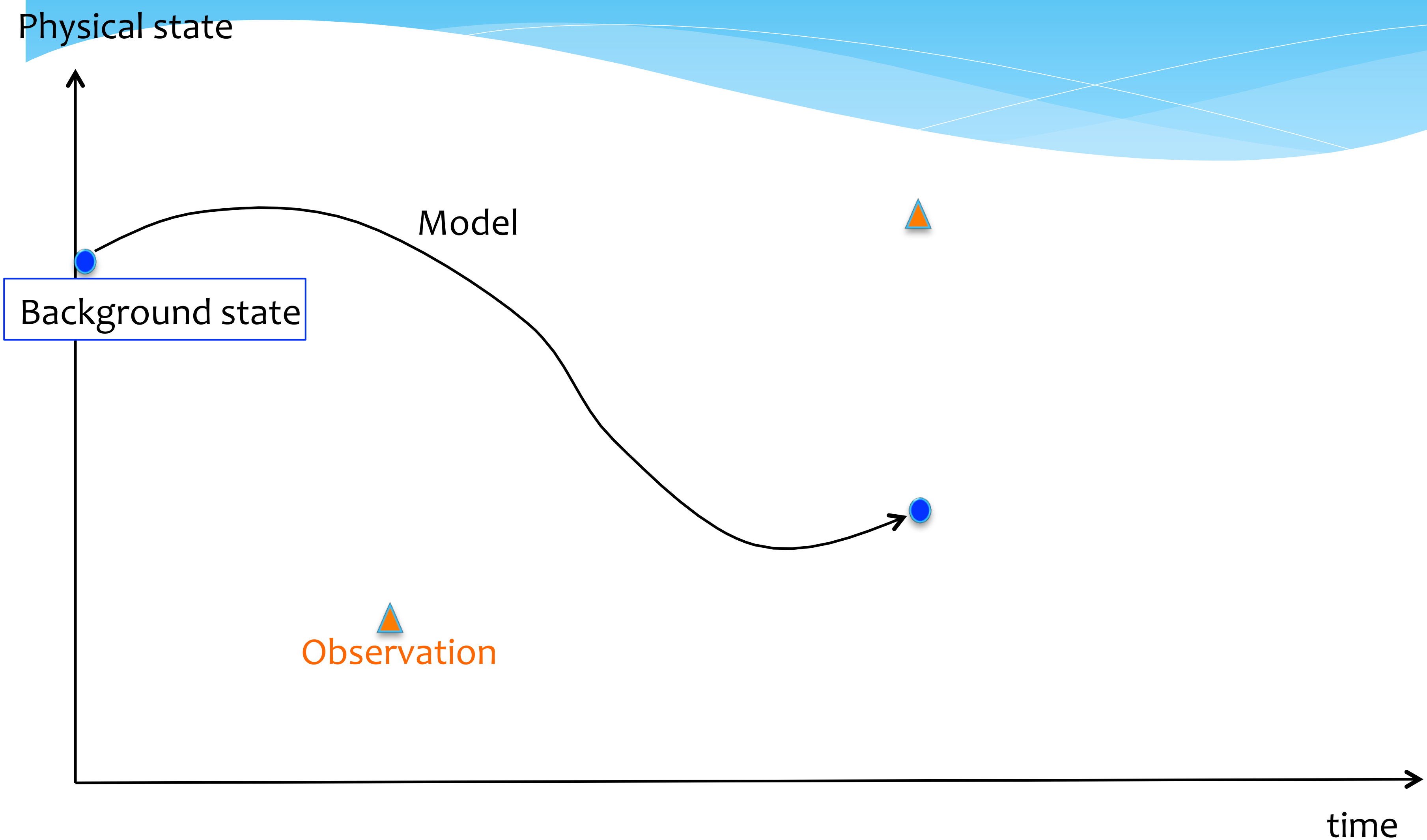
$$J_{4D}(x_0) = \frac{1}{2}(x_0 - x^b)^T\mathbf{B}^{-1}(x_0 - x^b) + \frac{1}{2}\sum_{i=0}^{N}(H(M_{0\to i}(x_0)) - y_i)^T\mathbf{R}^{-1}(H(M_{0\to i}(x_0)) - y_i)$$

* Efficient minimisation algorithms are iterative and require the gradient $\nabla J(x_0)$
* Adjoint methods are (by far) the cheapest ways to compute the gradient at each iteration.
* The adjoint model is often 2-4 times more expensive than the direct model.

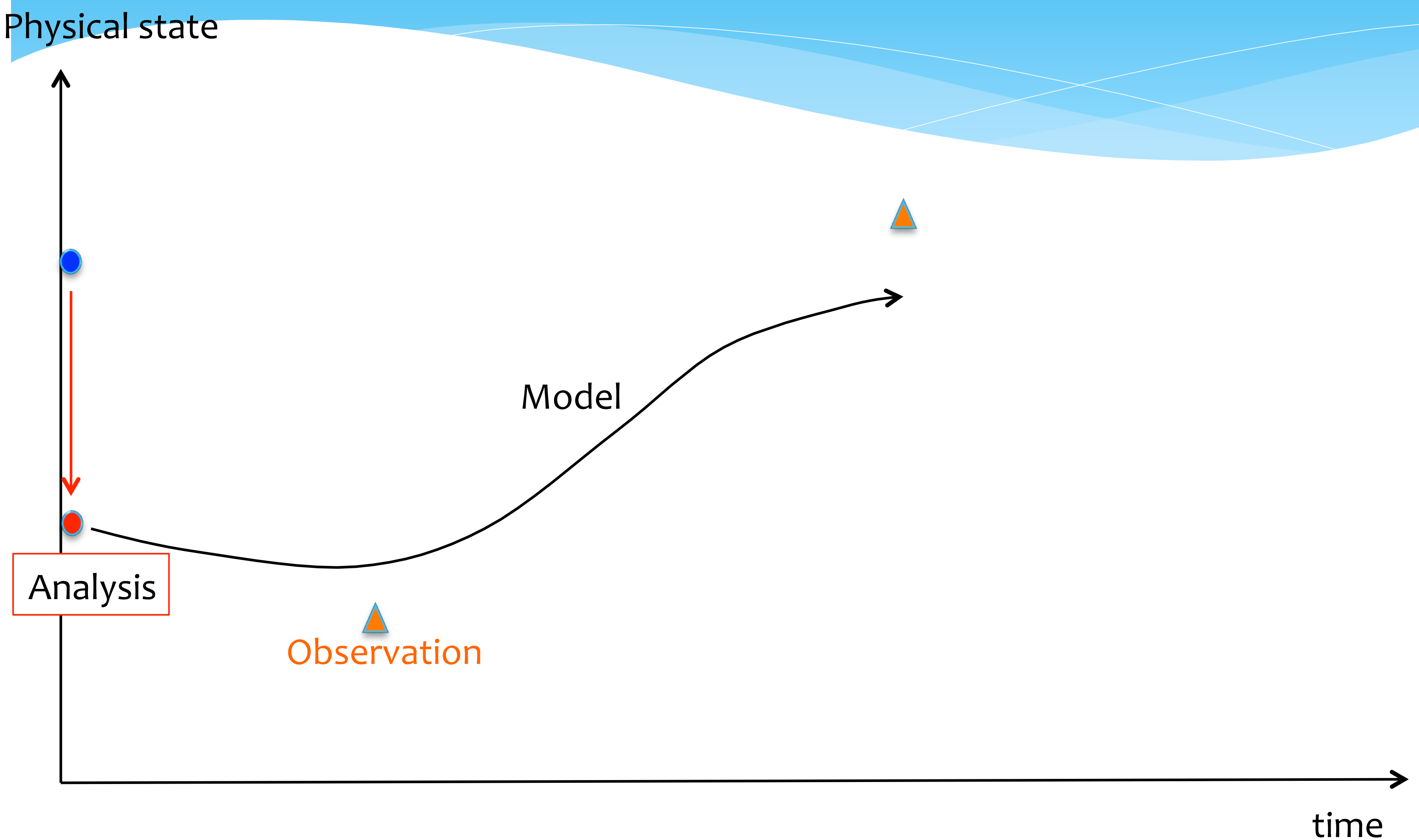
Variational methods



Variational methods



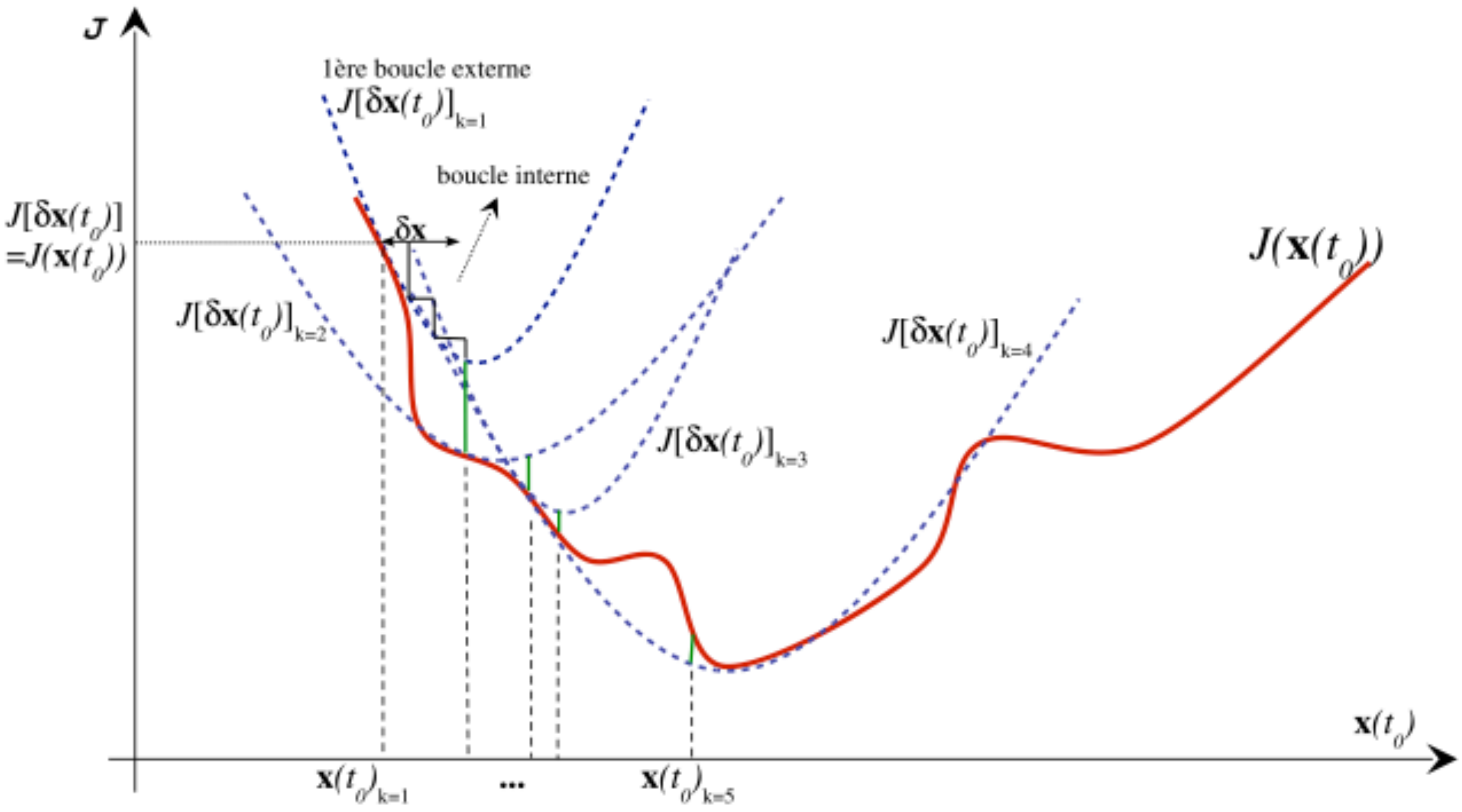
Variational methods



Incremental 4DVar

* When the model is non-linear, the cost function can be non-convex.
* Incremental 4D-Var splits the minimisation problem into a series of minimisations of quadratic (convex) cost functions.
* This leads to define outer and inner loops in the minimisation process.

Incremental 4DVar



Parameterization of the covariance matrix

* As with the EnKF, the full covariance matrix cannot be built and stored.

Parameterization of the covariance matrix

* A reduced-rank approach can be considered.
* The 4DVar increment is searched as a linear combination of a fixed set of error modes:

$$\delta \mathbf{x}_0 = \sum_{i=1}^{r} w_i \mathbf{L}_{\{i\}} = \mathbf{L}\mathbf{w}$$

* Minimization is carried out on **w**, a vector of size r.

(Robert et al, 2005)

Parameterization of the covariance matrix

Experiment with a Tropical Atlantic model and 1 observation of T. Figure shows the increment in T.

Maximal correction is
0.94 on top
0.06 on bottom

The observation is here

Vertical section

Full 4DVar (diagonal B)

Reduced rank 4DVar

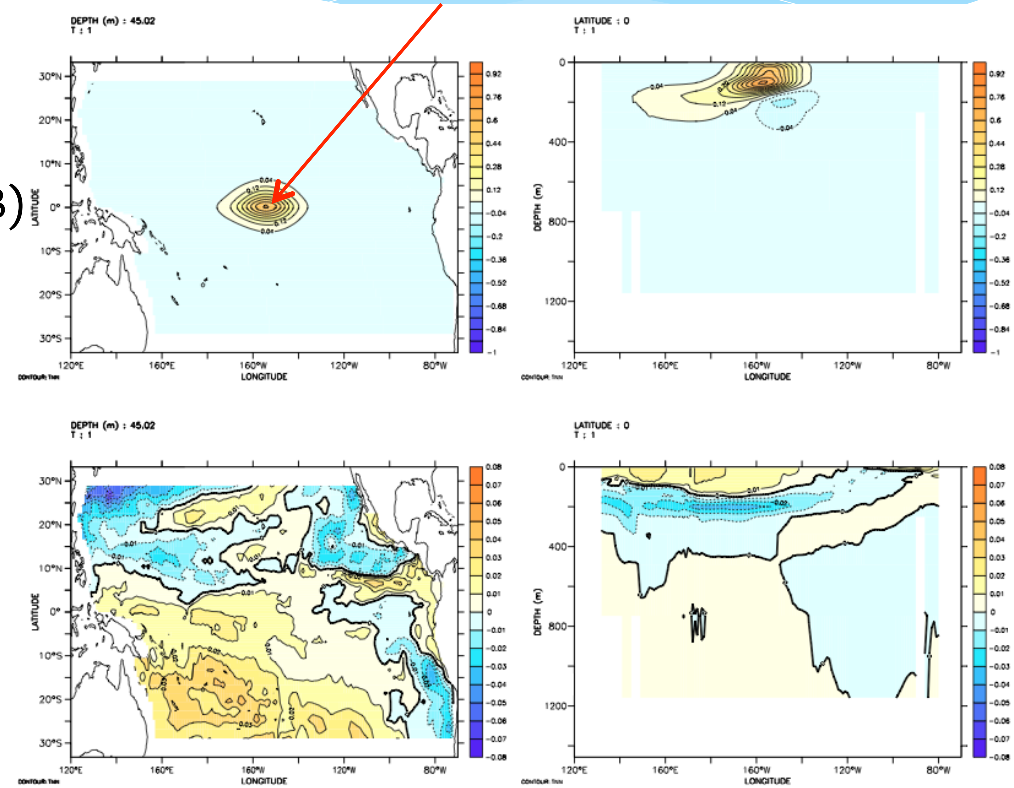


Fig. 4. Temperature component of the optimal increment δx_0 for single observation experiments. Left: horizontal structure at $z = -45$ m; right: vertical section along the equator. Top: full-space 4D-Var; bottom: reduced-space 4D-Var.

(Robert et al, 2005)

Parameterization of the covariance matrix

* Modelling of the covariance matrix with a suite of perators:

$$B = KD^{1/2}C^{1/2}(C^{1/2})^T D^{1/2}K^T$$

with

* K: balance operator
* D: variances (diagonal)
* C: correlations (block diagonal), built with a diffusion operator

(Weaver et al, 2005)

Parameterization of the covariance matrix

* The balance operator is introduced to form uncorrelated variables from the physical variables:

$$(T, S, SSH, U, V) \xrightarrow{K^{-1}} (T, S_U, SSH_U, U_U, V_U)$$

* The uncorrelated variables are then used in the control vector.
* The uncorrelated (unbalanced) variables are formed by removing their parts that are balanced by the others.

(Weaver et al, 2005)

Parameterization of the covariance matrix

A single obs of T, located at 160W, 0N, 100 m depth. 10-day 4DVar increments on SSH, without (left) and with (right) the balance operator.

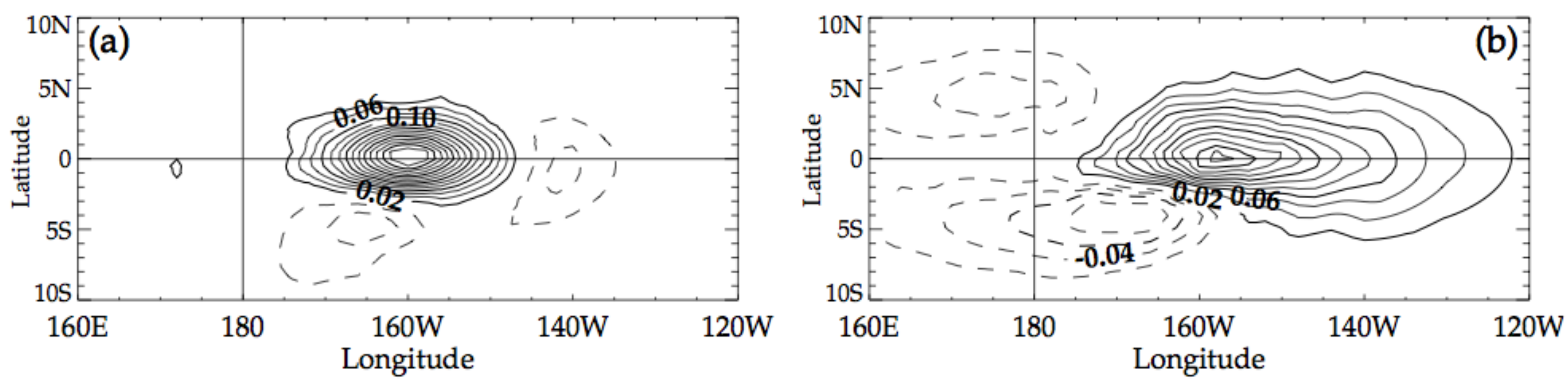


Figure 4. Horizontal section of the SSH analysis increments generated by the 4D-Var assimilation of a single-temperature observation (positive innovation) located ten days into an assimilation window at the same geographical location as in the example in Fig. 2. The increments are displayed on day 10 for a 4D-Var experiment (a) without and (b) with the balance operator activated. The fields have been multiplied by a factor 100 and the same contour interval has been used here as in Fig. 2(e). Solid (dashed) contours indicate positive (negative) values.

(Weaver et al, 2005)

Mercator-Océan operational DA system

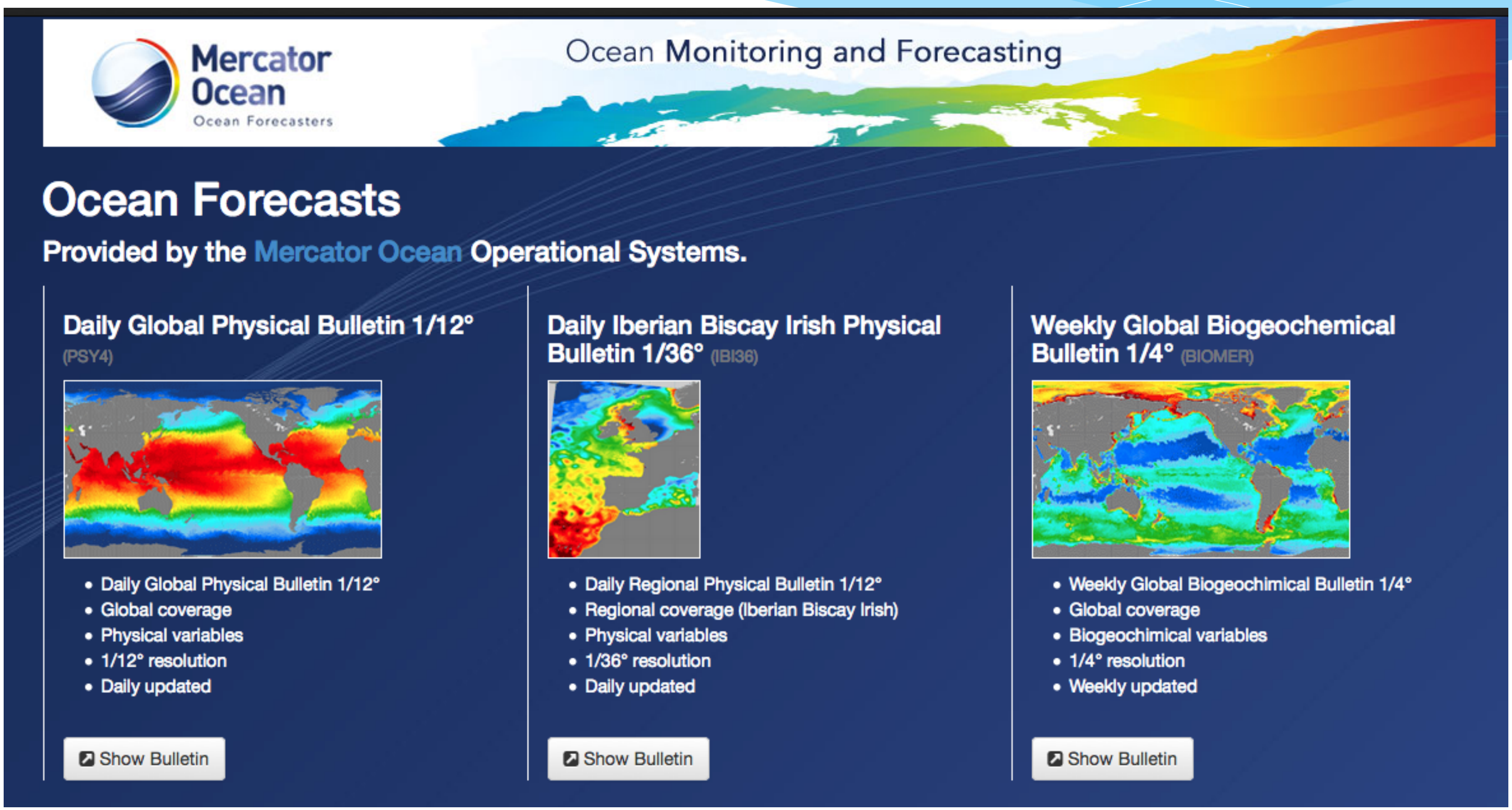
* Input from <u>**C.-E. Testut**</u>, O. Legalloudec, J.-M. Lellouche, L. Parent, E. Remy *(Mercator-Ocean)*, M. Benkiran, E. Greiner, B. Tranchant *(CLS)*

Mercator-Océan operational DA system

- System overview
- Covariance matrix
- Bogus
- Localization
- IAU
- Some perspectives

Mercator-Océan DA system

System overview

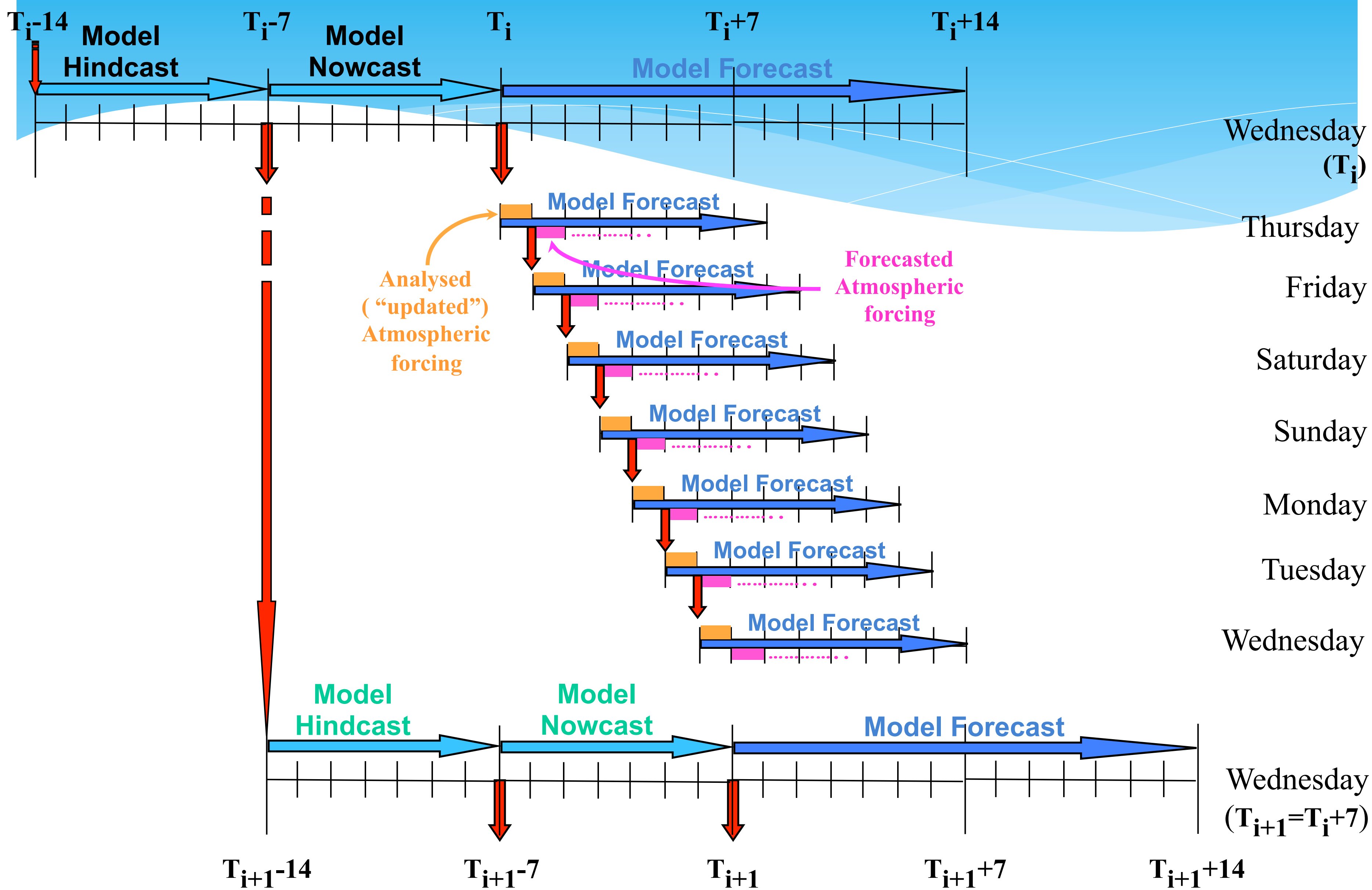


System overview

* The current global system
  * ORCA12 (1/12°) (NEMO 3.1 code)
  * SEEK (EnOI, RRSQRT filter with fixed error basis)
  * 3D-Var slowly evolving large-scale T/S bias correction
  * IAU
* Assimilated Data
  * SLA (DUACS)
  * “AVHRR+AMSRE” SST
  * T/S vertical profiles from CORIOLIS data center

Mercator-Océan DA system

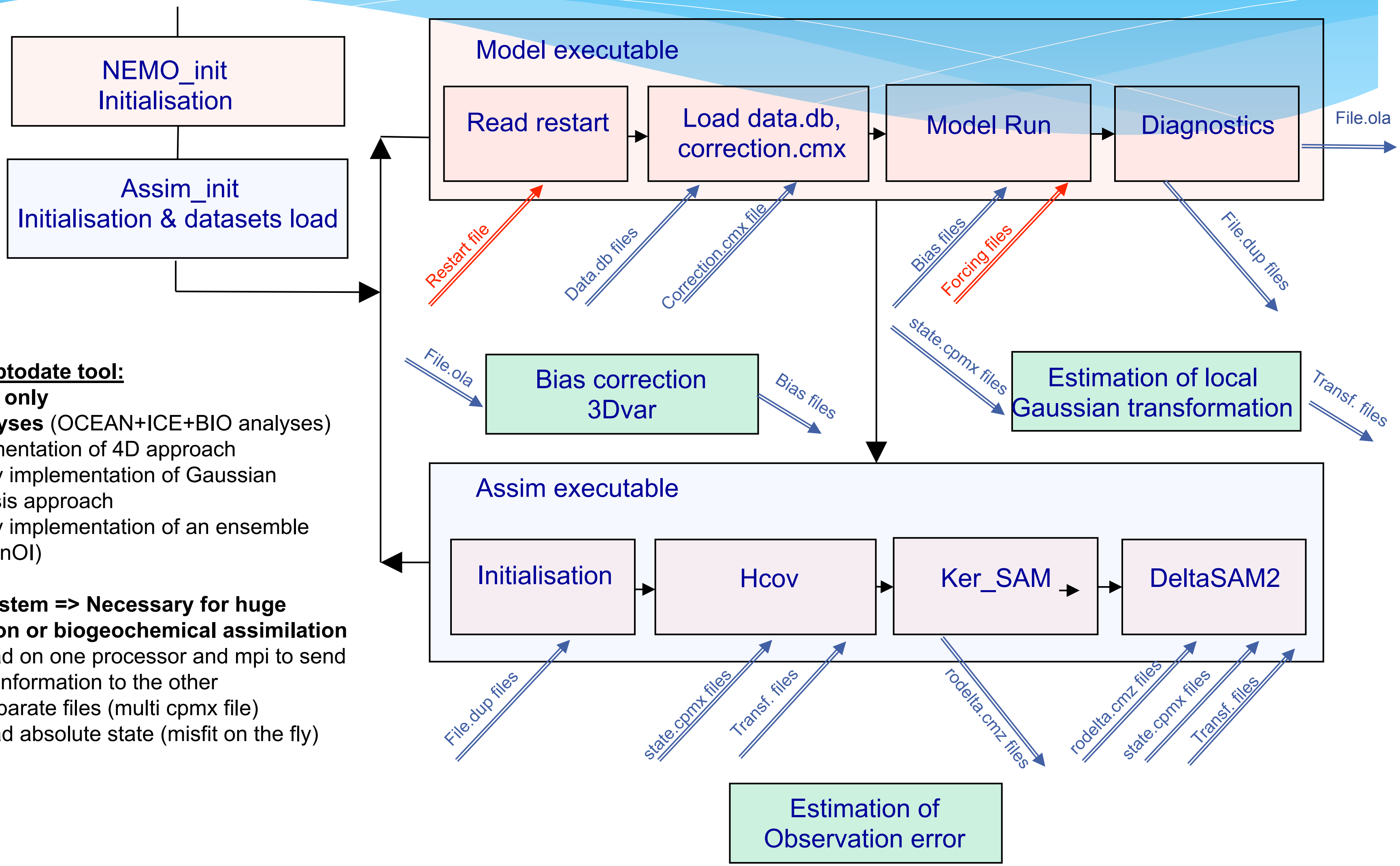
System overview



Mercator-Océan DA system

System overview

SAM2V2_uptodate platform



<u>SAM2V2_uptodate tool:</u>
- **Ksh chain only**
- **multi analyses** (OCEAN+ICE+BIO analyses)
- Full implementation of 4D approach
- Preliminary implementation of Gaussian anamorphosis approach
- Preliminary implementation of an ensemble approach (EnOI)

- **New IO system => Necessary for huge configuration or biogeochemical assimilation**
  - load on one processor and mpi to send the information to the other
  - separate files (multi cpmx file)
  - load absolute state (misfit on the fly)

System overview

* The analyses are performed using an ETKF kernel:

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

With $\Gamma = (\mathbf{H}\mathbf{S}^f)^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{S}^f)$

* with a fixed basis of error, IAU, localization, bogus

System overview

* The control vector is composed of:
  * Temperature, Salinity, U, V
  * Sea ice concentration
  * SSH, HBAR (barotropic component of SSH), and HBRST (temporal and spatial smoothing of HBAR)

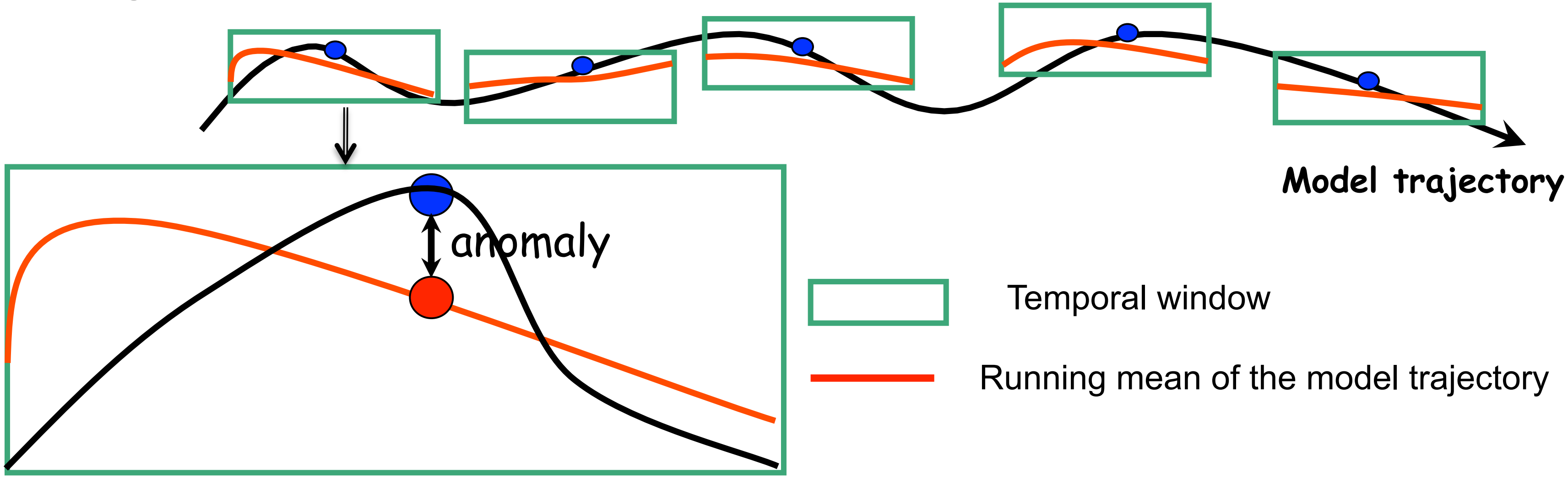
HBAR and HBRST are involved to circumvent the fact that the assimilated SLA does not contain any information about the mean ocean circulation.

Mercator-Océan DA system

Covariance matrix

* Construction of the error basis.

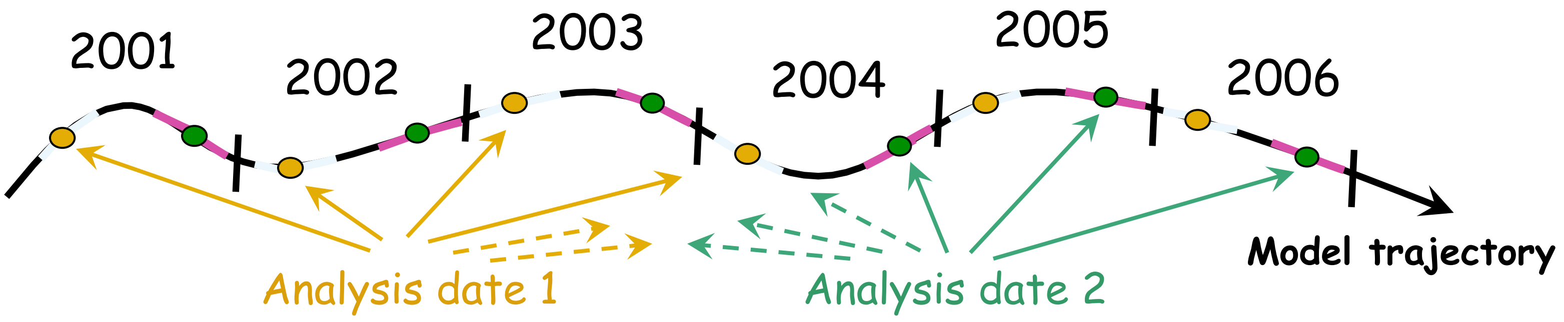
➢ **We generate a pseudo-ensemble from a forced simulation**



Covariance matrix

* Construction of the error basis.

➢ **We use these anomalies to compute Pf in the analysis**



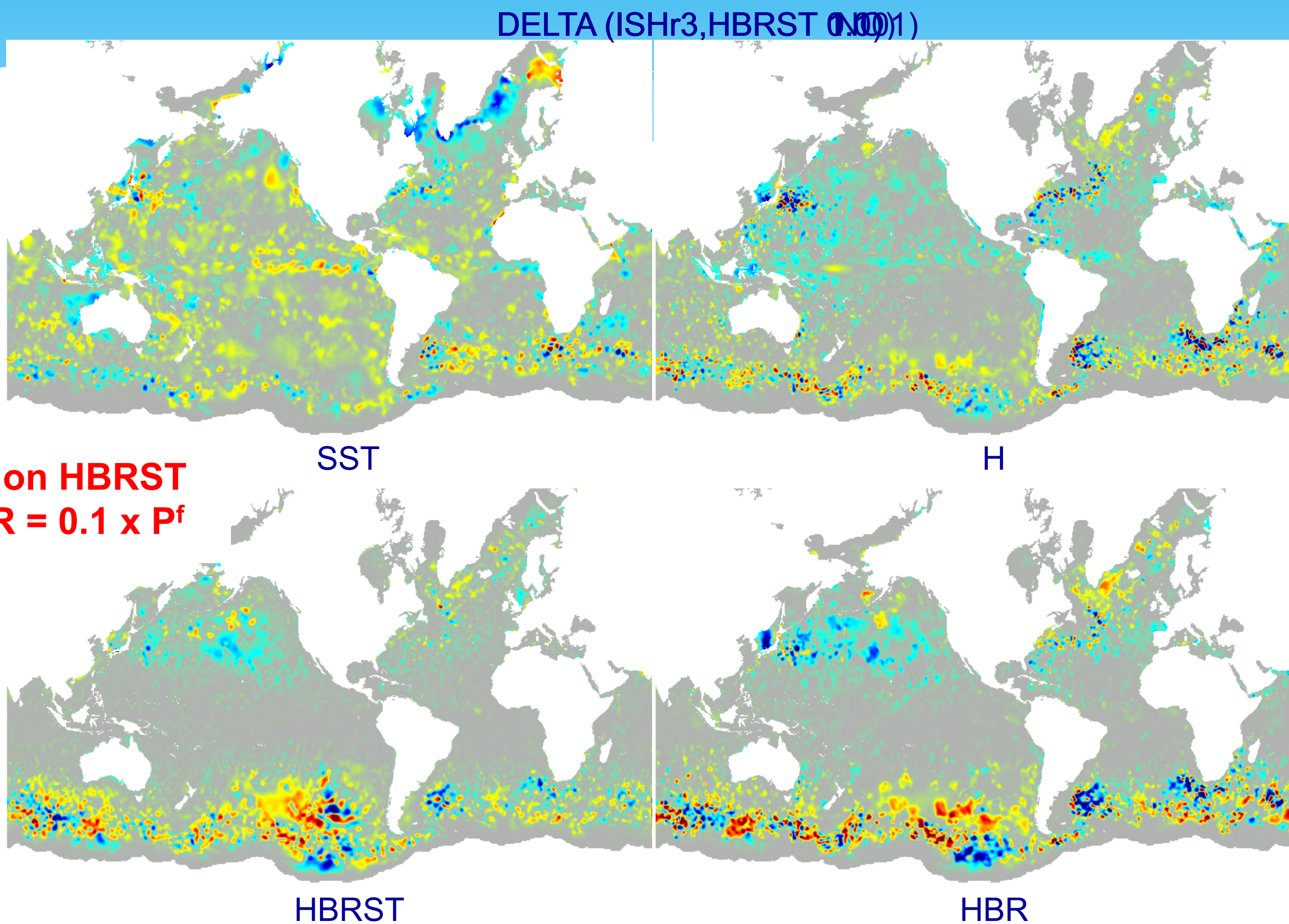
And some adaptive adjustment of the forecast error variance at each assimilation cycle in order to be consistent with innovation statistics.

Bogus

* Bogus (forced null innovation with R= coef x Pf):
  * HBRST (strong constraint)
  * Salinity (Run Off)
  * HTSUV (under ice)
  * TSUV (Tropic)

Mercator-Océan DA system

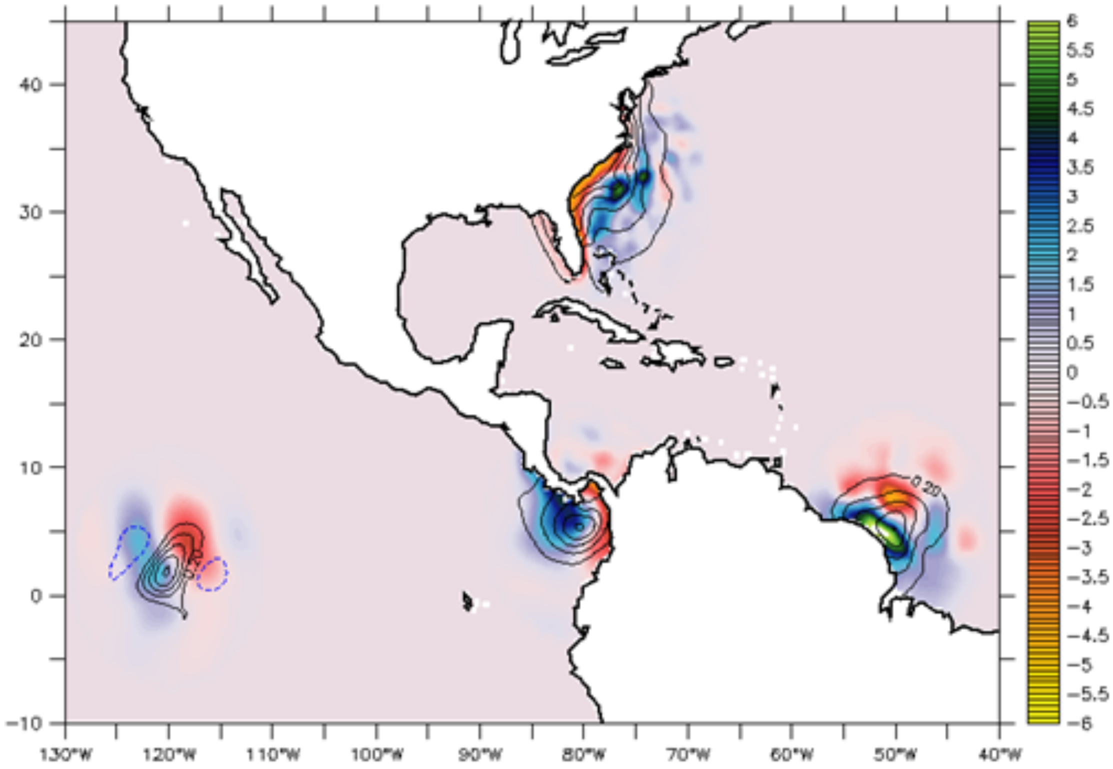
Bogus



Bogus on HBRST using R = 0.1 x P^f

Mercator-Océan DA system

Localization

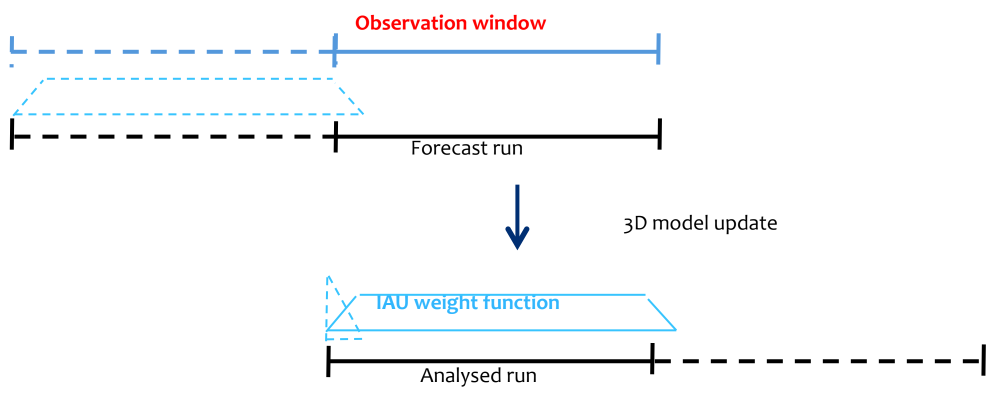


4 independent representer of height (color) and SST (isoline) for 4 single SST innovation of 1°C

Mercator-Océan DA system

IAU

* IAU is run over 8 days;
* The weight function
  * Increases during 1 day,
  * Is constant during 6 days,
  * Decreases during 1 day.



Some perspectives

* Move towards an ensemble approach to
  * Increase efficiency
  * Provide probabilistic forecasts

* Upgrade of the model: Global 1/36, 100000 processors, 100 millions of observation, 100 000 observations for each local bubbles

* New schemes for sea ice, biogeochemistry

Future challenges

* Towards the use of higher resolution models
* Modeling the model error with stochastic parameterizations
* SWOT
* Assimilation of images

Towards the use of higher resolution models

* High resolution = high CPU cost = difficulties to run ensembles
* High resolution = more nonlinearities = more small-scale processes = more degrees of freedom = larger ensembles needed
* More nonlinearities = need for nonlinear DA methods, much more expensive
* At present, most part of the gain in machine capacity is allocated to increase models resolution.

Modeling the model error with stochastic parameterizations

* Stochastic parameterizations emerge as an essential tool for representing uncertainties in models, hence for DA.
* But the set-up can be challenging.

Modeling the model error with stochastic parameterizations

* Stochastic parameterizations emerge as an essential tool for representing uncertainties in models, hence for DA.
* But the set-up can be challenging.

Modeling the model error with stochastic parameterizations

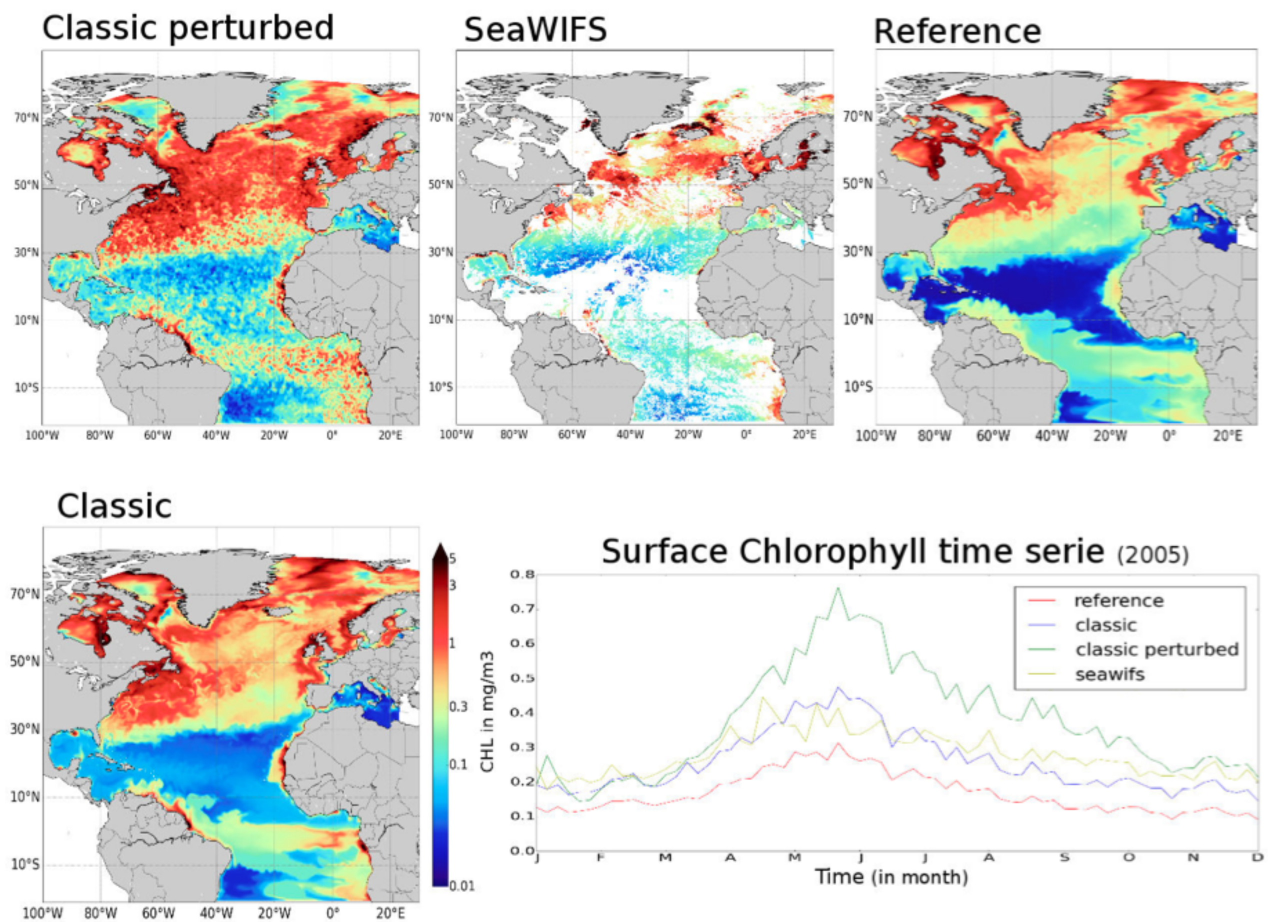
Example:
Ensemble of simulations of the biogeochemical cycle in the North Atlantic
Perturbation of 7 parameters (phyto growing rate, grazing rate, etc) around the values prescribed originally in the "deterministic" model.

$$\frac{\partial c_i}{\partial t} + \boldsymbol{u}.\nabla^h c_i + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial z}\left(\tilde{\lambda}\frac{\partial c_i}{\partial z}\right) + S(c_i, c_j, \alpha_n)$$

(Garnier et al, in prep)

Modeling the model error with stochastic parameterizations

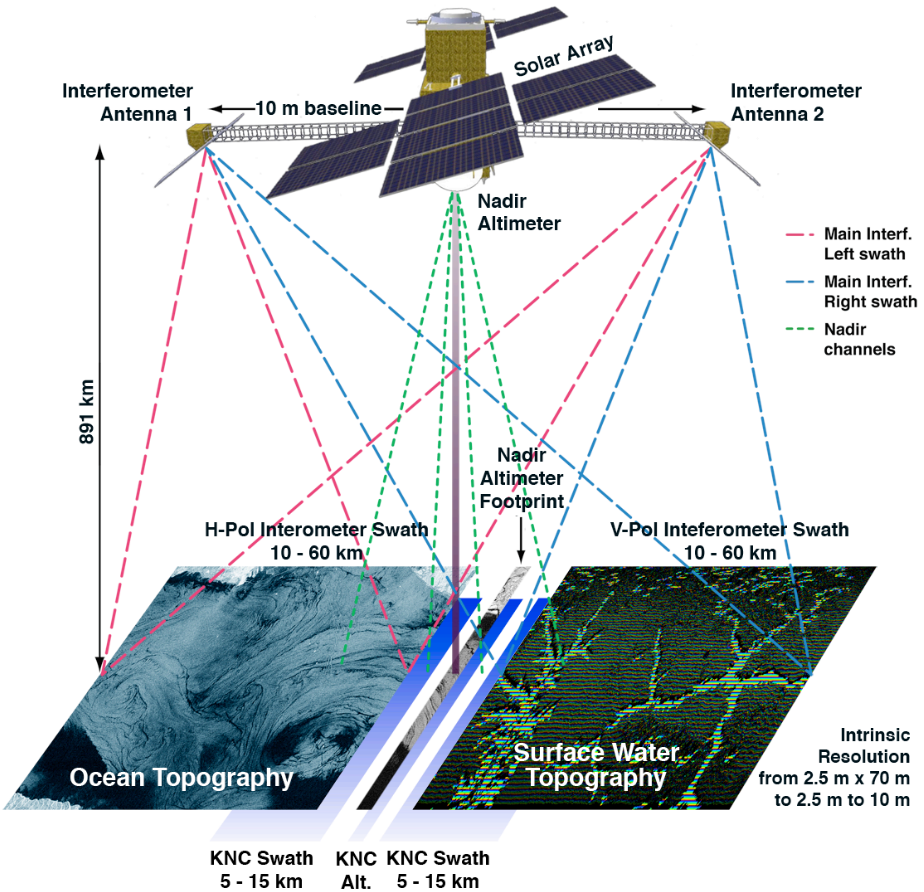
A correct representation of phytoplankton requires a full retuning of the reference parameters.



(Garnier et al, in prep)

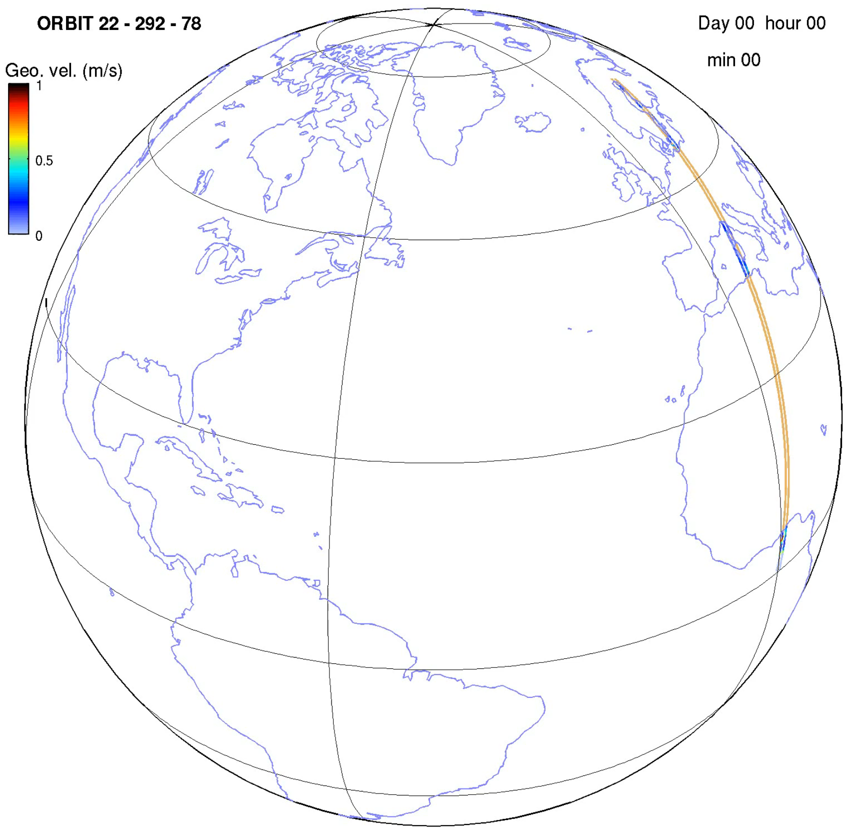
SWOT

* SWOT: Surface Water and Ocean Topography
* Satellite mission to be launched in 2021
* Revolutionary altimetric observation: 120 km-wide swath
* Pixel of 1 km



Future challenges

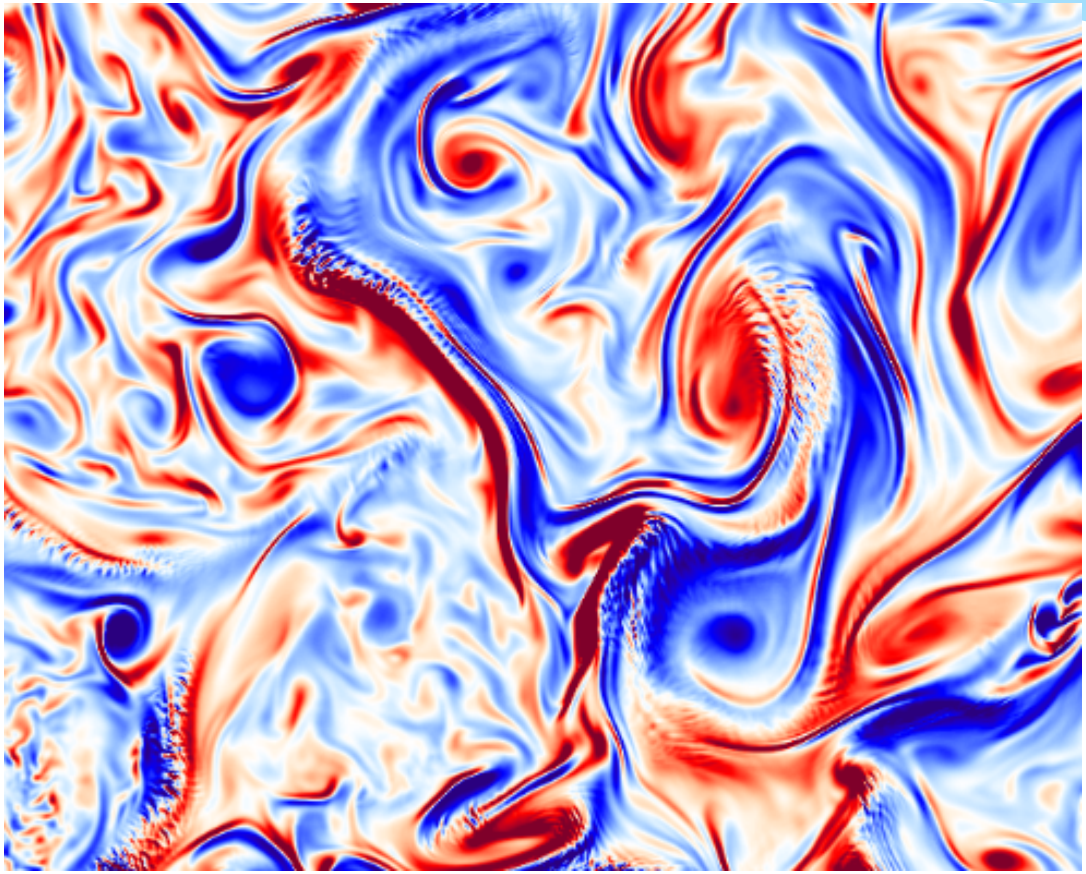
SWOT



SWOT

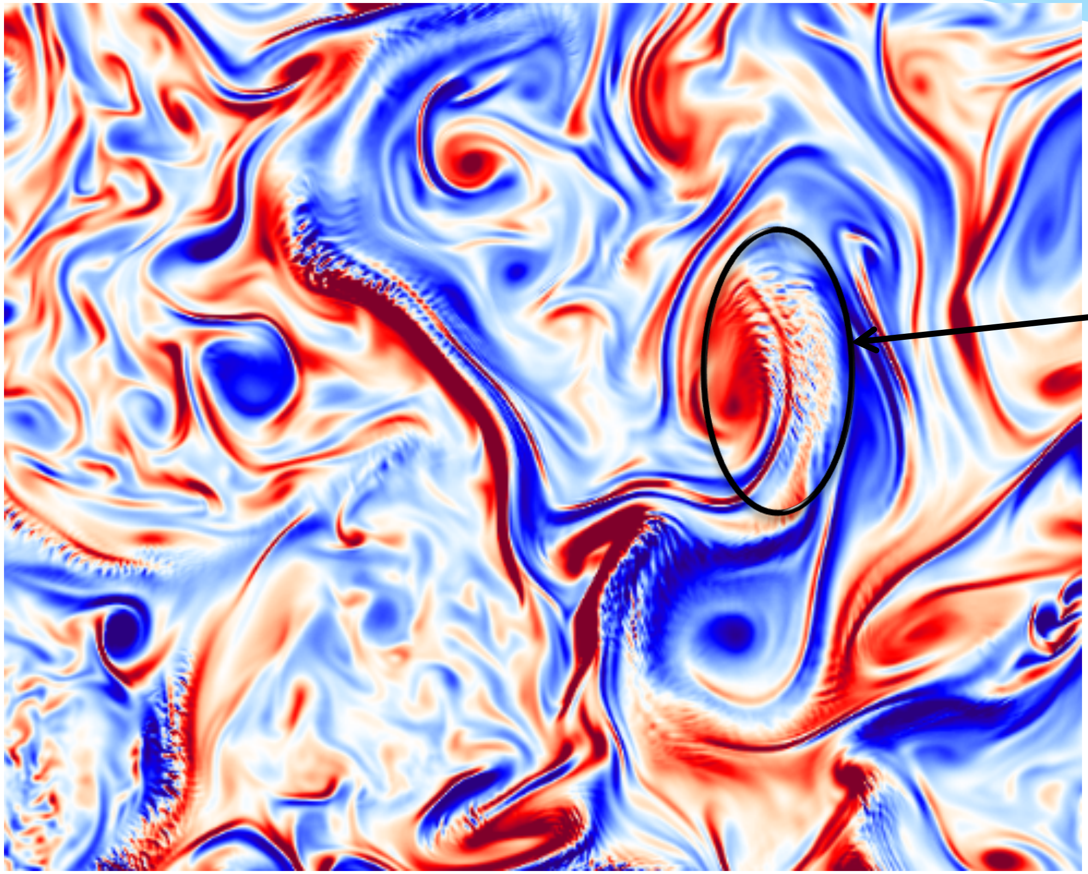
* Challenges:
  * The physical processes that will be observed are not well known;

SWOT



Snapshot of ΔSSH from the 1/60° North Atlantic simulation

SWOT



Physical processes or numerical artefact?

SWOT

* Challenges:
  * The physical processes that will be observed are not well known;
  * The signature of internal tides cam be superposed to the balanced dynamics;

Future challenges

SWOT

Phenomenon	Length scale L	Velocity scale U	Time scale T
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

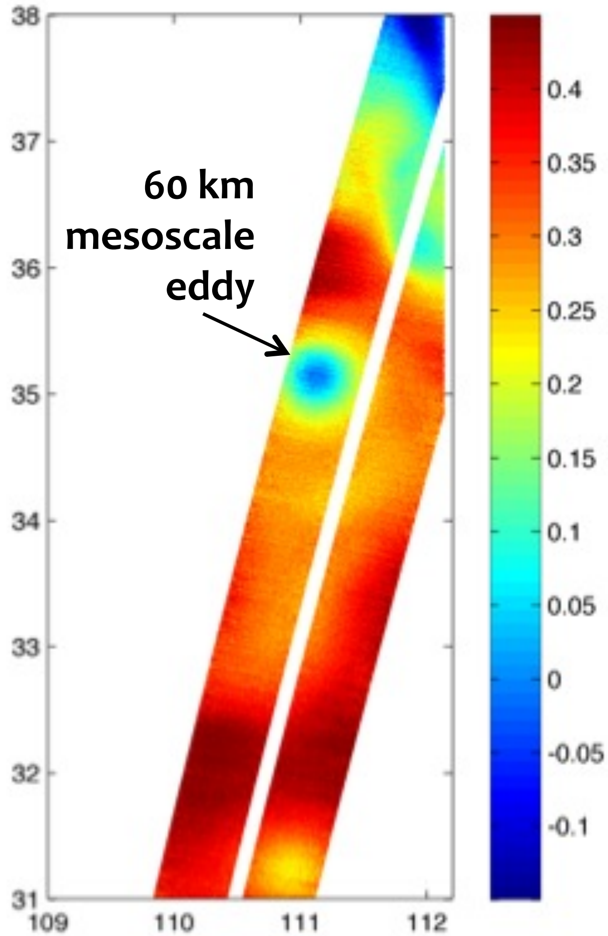
SWOT

Conventional nadir altimetry

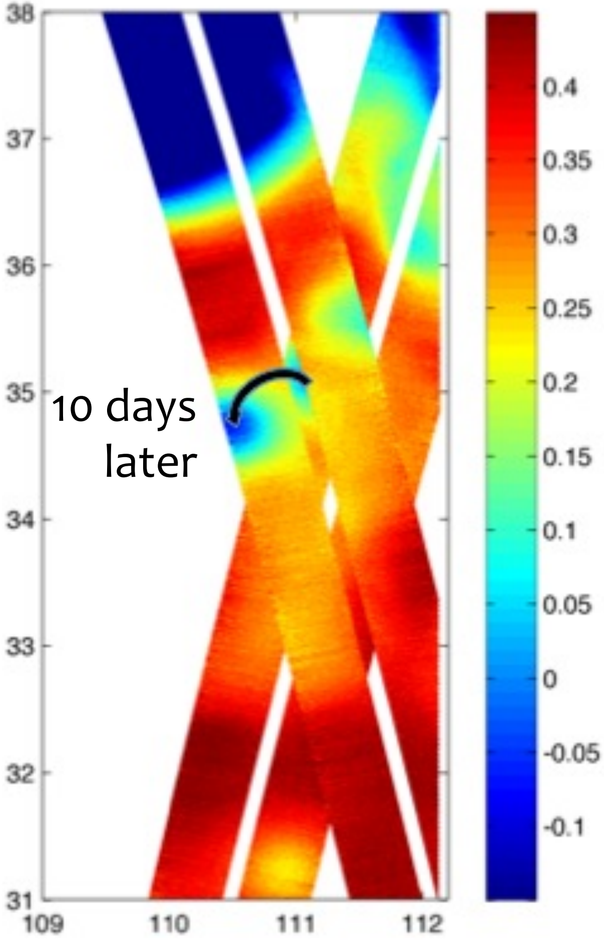
SWOT

- Challenges:
  - The physical processes that will be observed are not well known;
  - The signature of internal tides cam be superposed to the balanced dynamics;
  - The satellite will provide well separated (in time) snapshots of short-lived structures.

SWOT


60 km
mesoscale
eddy
38
37
36
35
34
33
32
31
109
110
111
112
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1

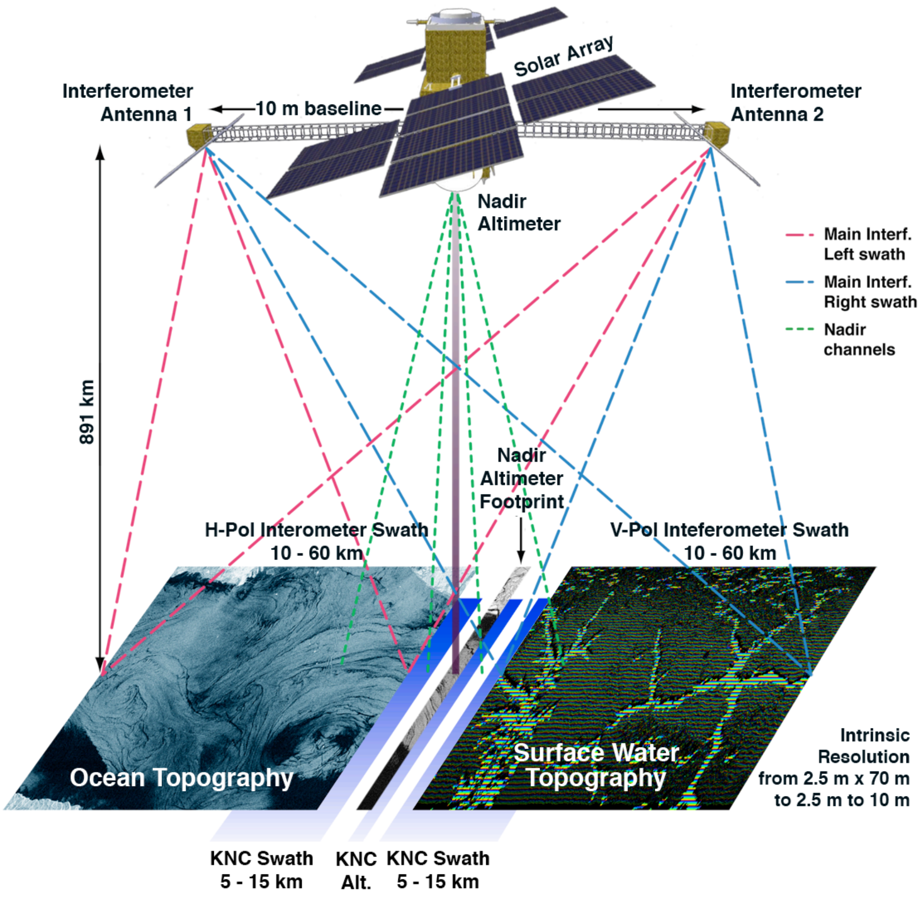
SWOT



Can we retrieve the SSH evolution between the two satellite revisits?

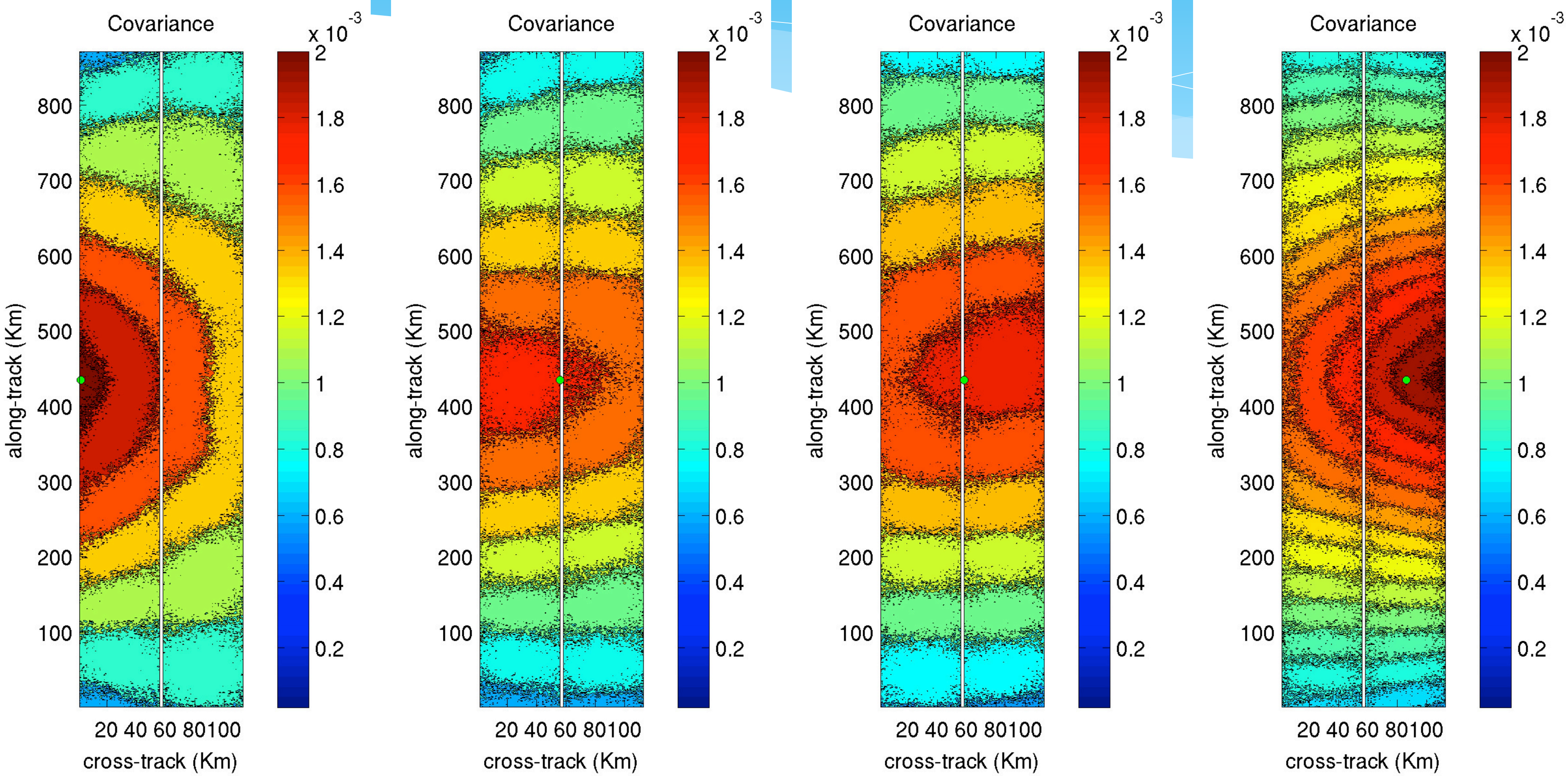
SWOT

* SWOT observations will be affected by correlated noise (due to roll, tropospheric water vapor, dilation of the baseline, etc)



Future challenges

SWOT



Error covariance fields from a simulator of the SWOT error.

Assimilation of images

* Images (here, chlorophyll) clearly reveal the structure of the flow;
* How can such data be assimilated into models as images?

Thank you

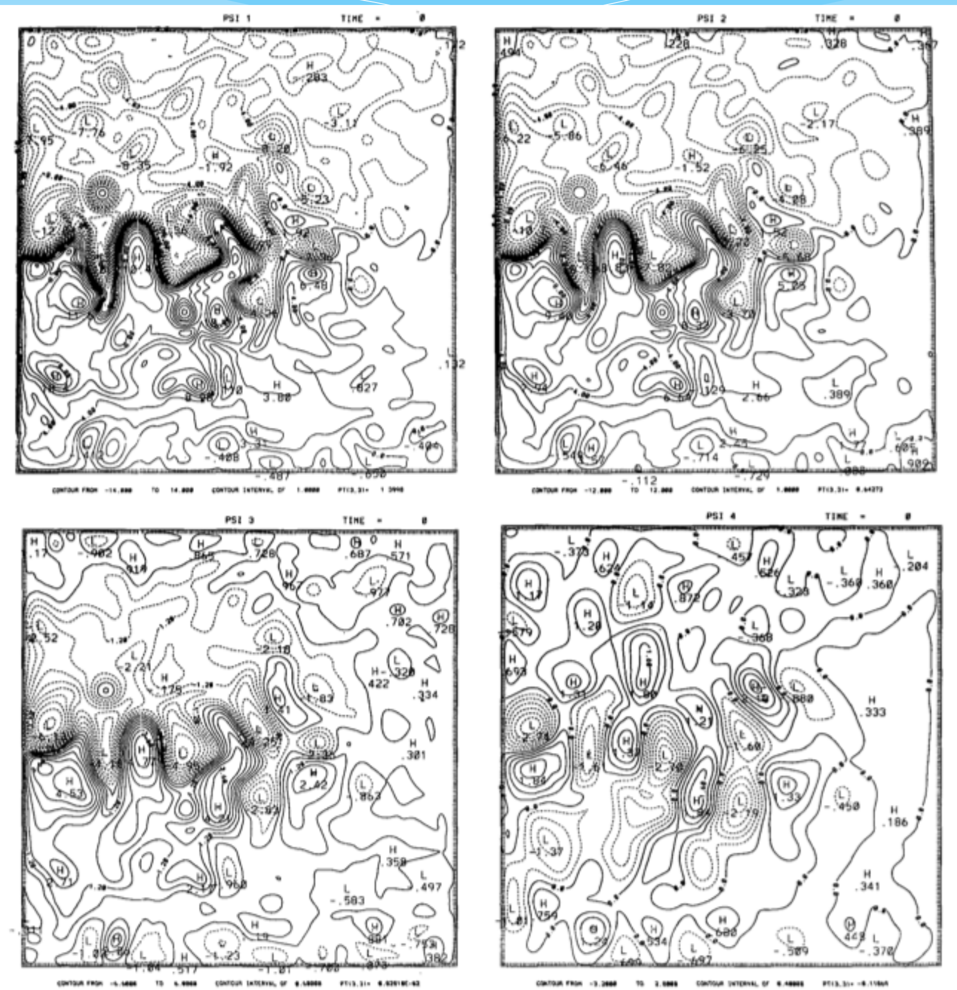
Vertical projection of altimetry

* Altimetry provides surface observations only.
* In an EnKF framework, it is natural to rely on the ensemble statistics to correct subsurface variables.
* There can be a limit to this: biases due to the mismatch between the time scales covered by altimetry and of the deep water masses.
* Dynamical projection, instead of statistical, can be considered.

Vertical projection of altimetry

Stream function fields from a 4-layer quasi-geostrophic ocean box model, layers 1 to 4.

One can expect obvious vertical correlations between these fields.



(Haines, 1991)

Vertical projection of altimetry

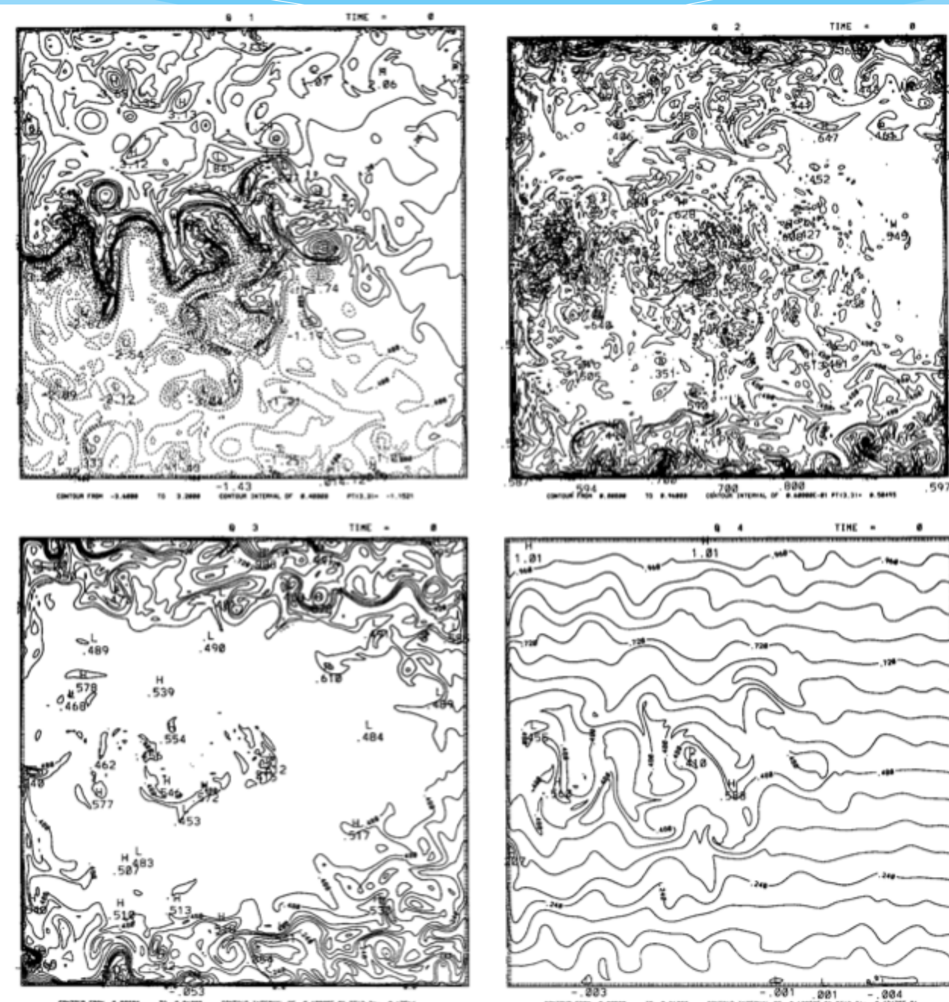
Potential vorticity from the same model, same time, same layers.

No clear relationship between layers.

But layer 1 is connected to stream function.

This suggests that subsurface potential vorticity should be conserved during the assimilation of altimetry (layer-1 stream function).

(Haines, 1991)



Vertical projection of altimetry

* Potential vorticity is:

$$q = \frac{f}{\rho_0}\frac{\partial \rho}{\partial z}$$

* Preserving PV means preserving the stratification.