

# Ocean Data Quality Control [and Assimilation]

Select and assimilate “good” observations  
while rejecting “bad” observations  
when “good” and “bad” are system-dependent

JCSDA Summer Colloquium on Data Assimilation

Summer 2012

Kayo Ide

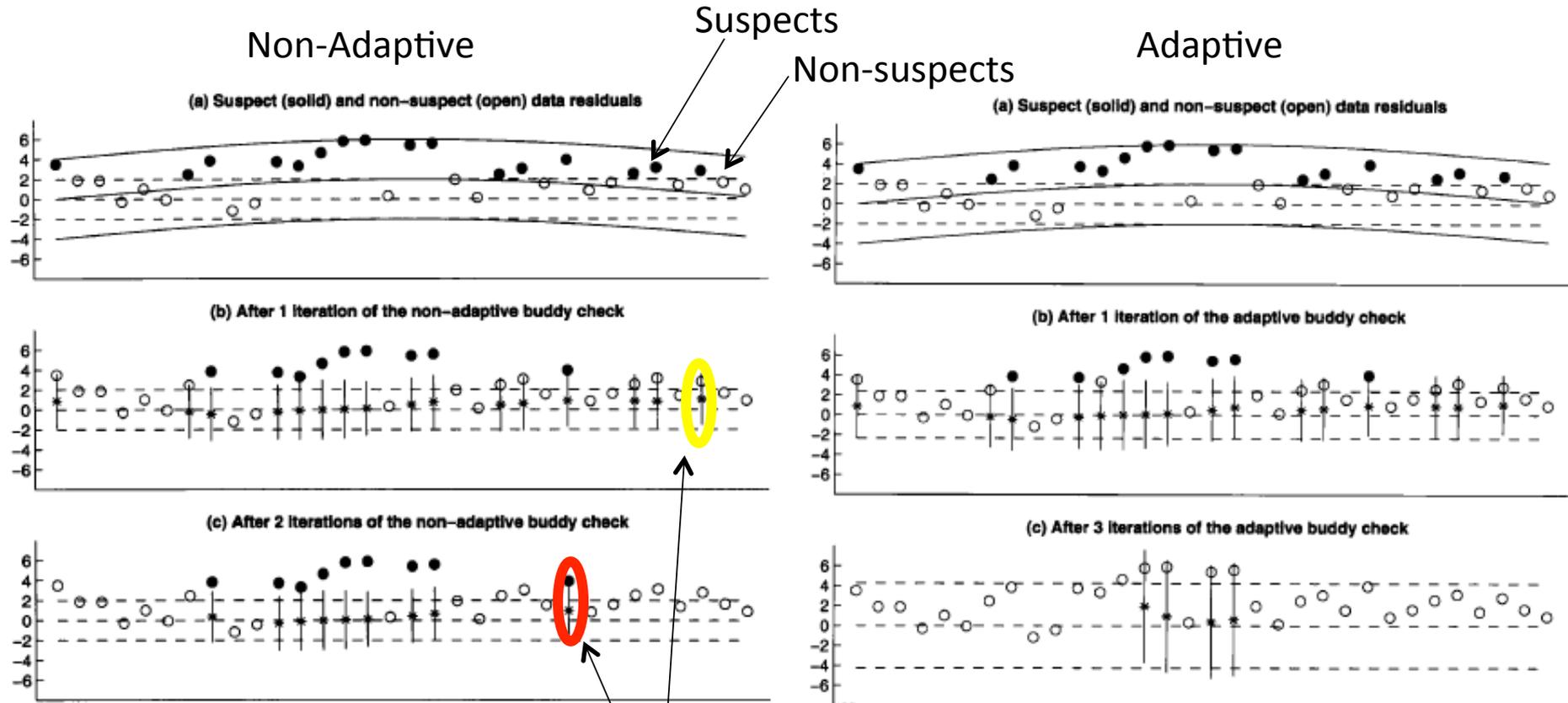
University of Maryland

# Basic Ideas for Ocean Data Quality Control

- ◆ Quality control (QC) for ocean data from data assimilation perspective
  - Basic concepts are similar to atmospheric systems from theoretical (Bayesian) view
    - If observations are abundant, then buddy check (not only to reject but also to accept)
    - If observations are sparse, primary corroborative source of information may be forecast (in particular in the form of ensemble)
  - Details may require unique adjustment, development, and implementation
    - Ocean data (network) can be sparse/inhomogeneous and sporadic
      - » If erroneous values are assimilated, then they can cause immediate spurious overturning and/or be advected around for years afterwards (nothing else to correct)
    - Ocean data assimilation is relatively new and may have different emphases from atmospheric data assimilation.
    - Scales are different in both:
      - » Dynamics
      - » Observations

# Background: Buddy-Check. Atmospheric Example

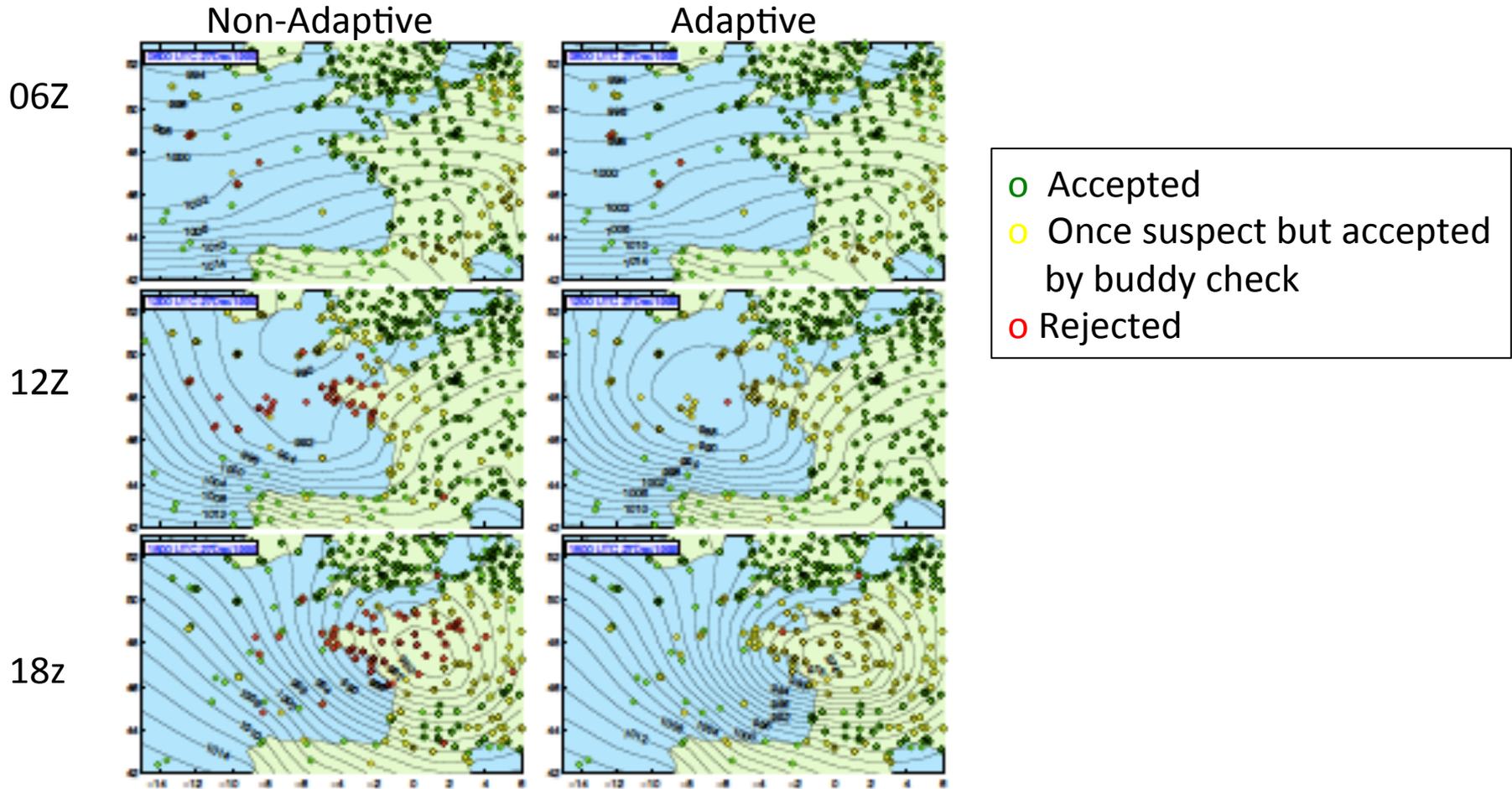
◆ Based on innovation  $\mathbf{d} = \mathbf{y}^o - \mathbf{h}(\mathbf{x}^b)$  for dense observing network



Given all non-suspects,  
 - conditional expectation  
 - conditional range with  $\sqrt{3\sigma}$

# Background: Buddy-Check

◆ Example: Intense storm over Europe December 27, 1999



*Dee et al (2001)*

# Outline

## ◆ Some examples of ocean data assimilation systems

- Global Operational & Reanalysis
  - Navy Coupled Ocean Data Assimilation (NCODA) [real time]
  - ECMWF ORA & ORT-S4 [re-analysis and real-time]
  - NCEP Global Ocean Data Assimilation system (GODAS) [real time]
  - Simple Ocean Data Assimilation (SODA) [reanalysis]
- Regional Operational/Real time
  - NCODA Relocatable system (RELO) [real time & Relocatable]
  - Southern California Coastal Ocean Observing System (SCCOOS) [near real-time]

## ◆ Types of ocean data used in the assimilation

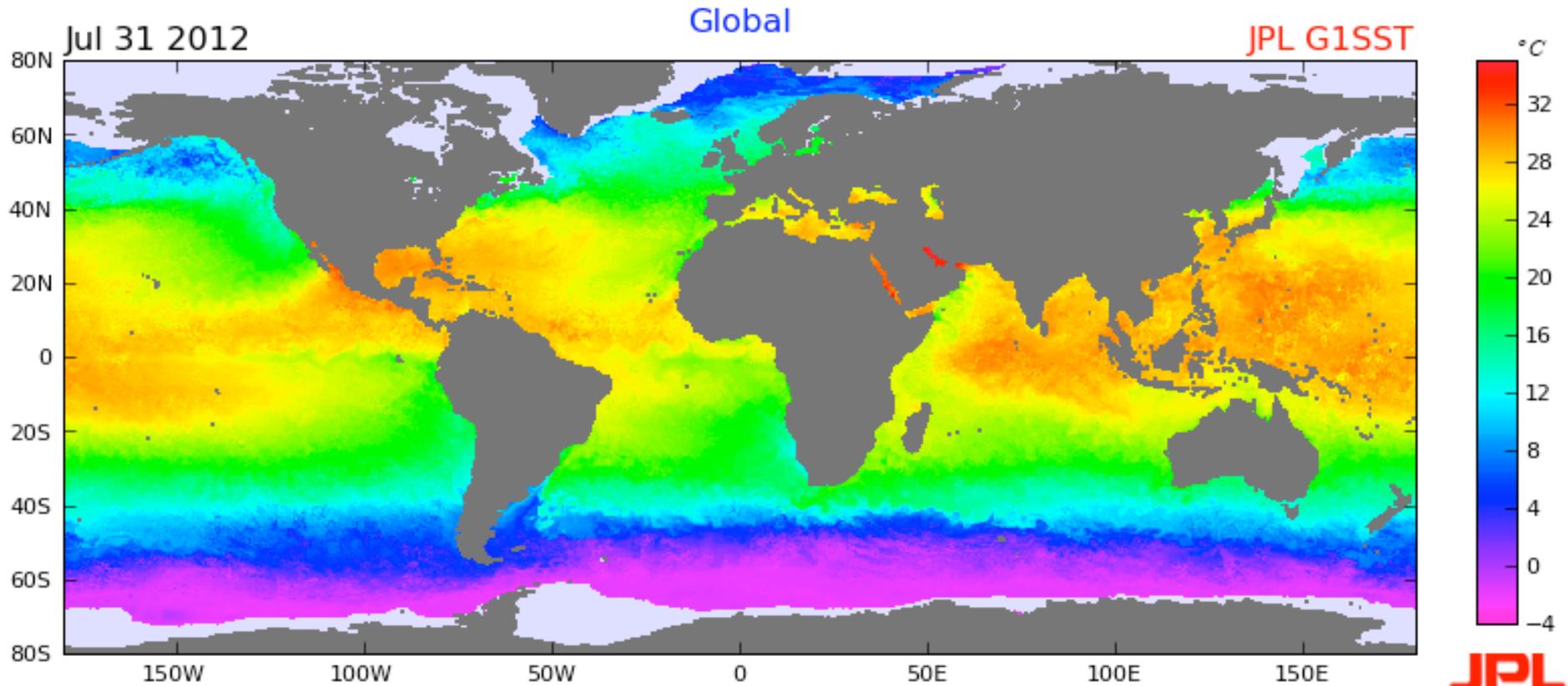
- Conventional platforms
  - In-situ [mainly T, S]
  - Remote sensing, satellite in particular, including Salinity
- New types of platforms
  - HF (high frequency) radar [surface (u,v)]
  - Lagrangian data [trajectories]

## ◆ Quality control

- Basic concepts
- Examples
- New perspective

# Ocean Observation: Satellite

## ◆ Sea Surface Temperature

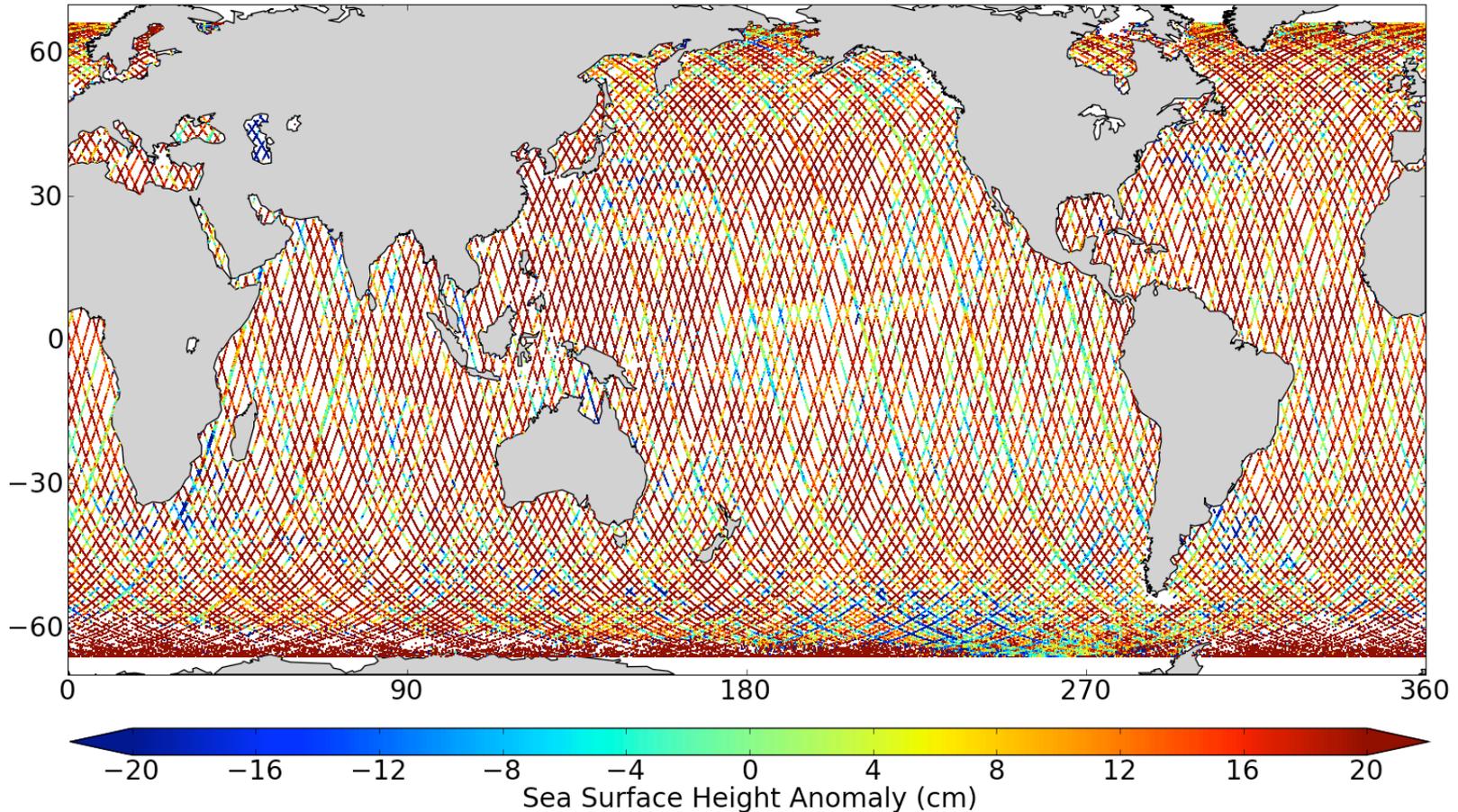


<http://ocean.jpl.nasa.gov/SST/#>

# Ocean Observation: Satellite

## ◆ Sea Surface Height

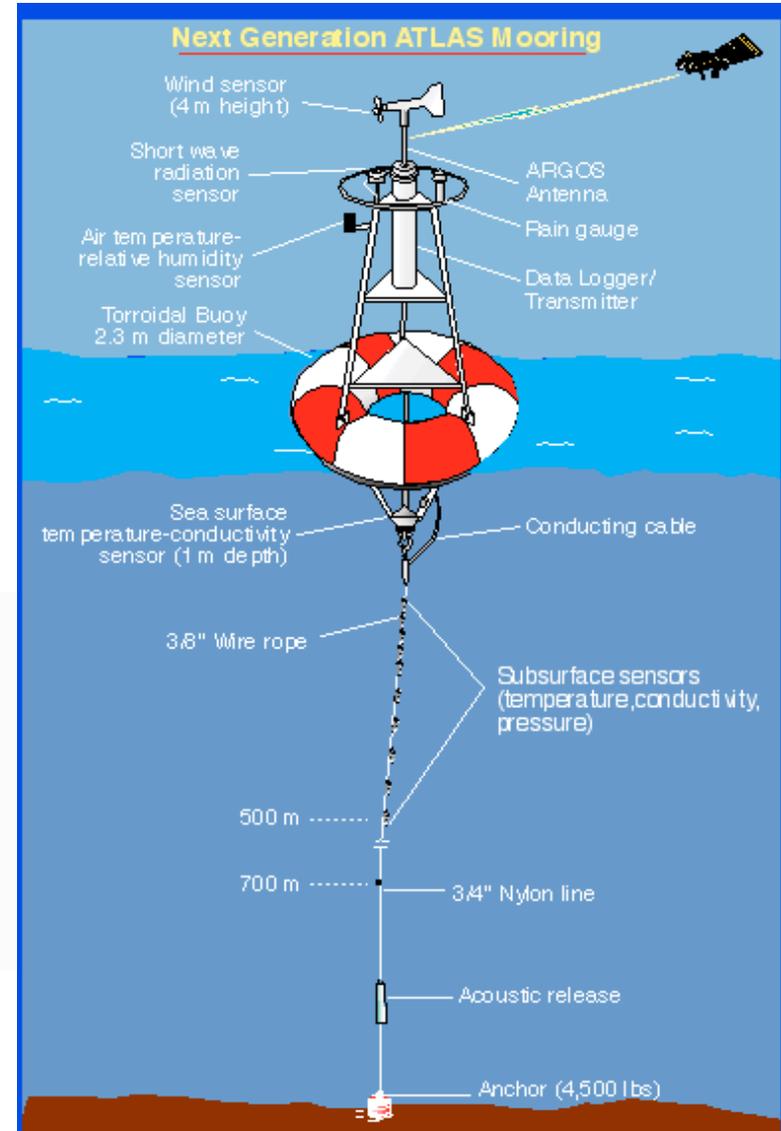
Sea Surface Height Anomaly: Jason-1 and Jason-2 Measurements from 23-Jul-2012 to 02-Aug-2012



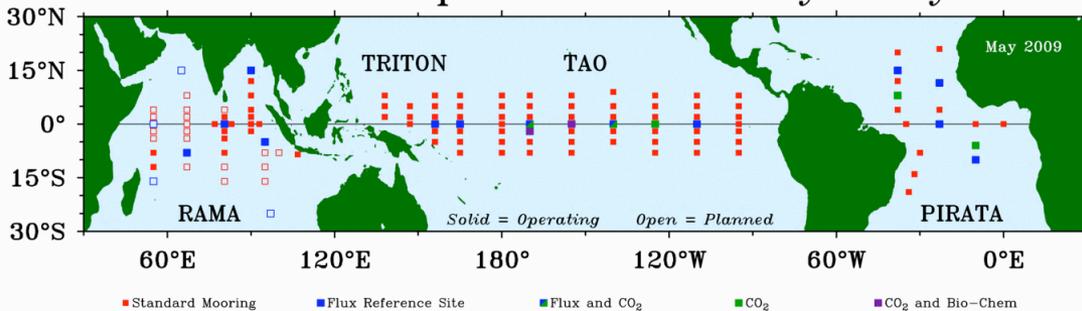
<http://sealevel.jpl.nasa.gov/Science/datasources/ssha/>

# In-Situ Instrument. Profiling Station

- ◆ Mooring: CTD, Surface observations
  - TAO (Tropical Atmosphere Ocean):  
For improved detection, understanding and prediction of El Niño and La Niña.
  - TRITON
  - PRITA (small no of deep water buoys)



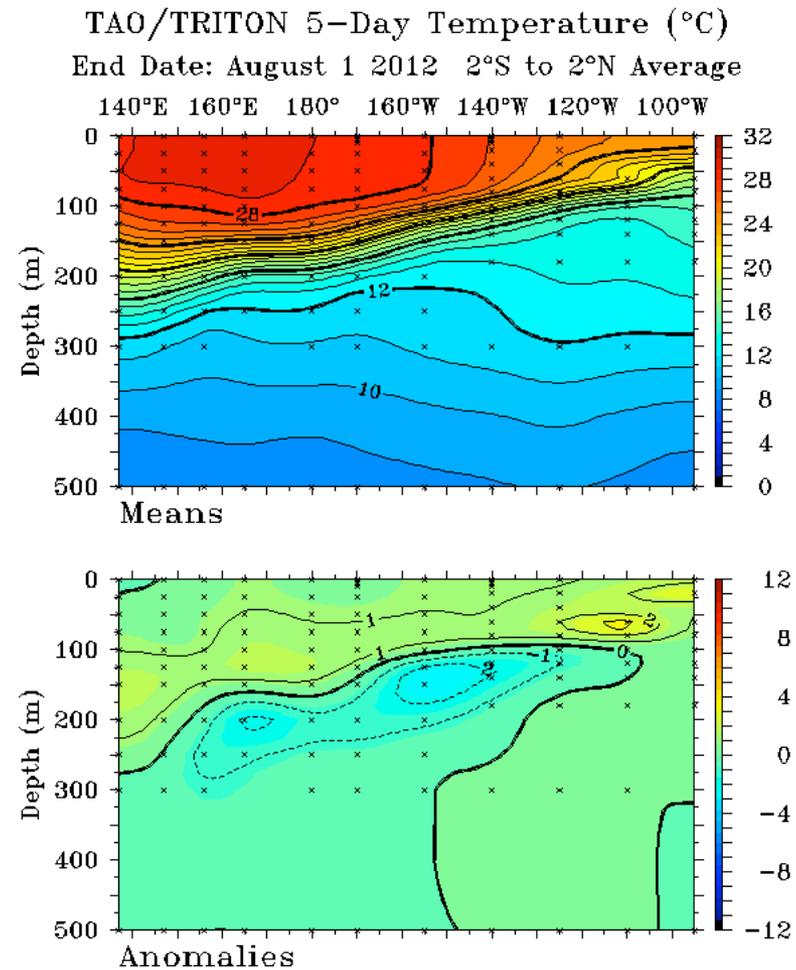
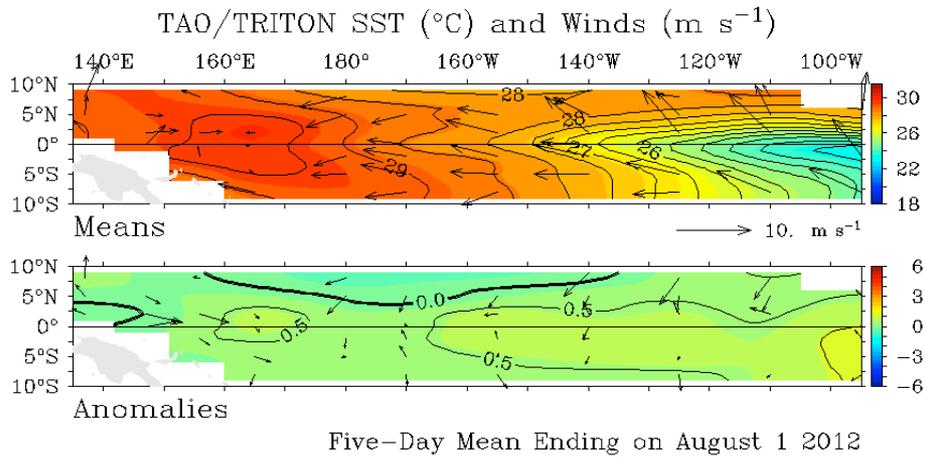
Global Tropical Moored Buoy Array



<http://www.pmel.noaa.gov/tao/index.shtml>

# In-Situ Data

## ◆ Mooring Data

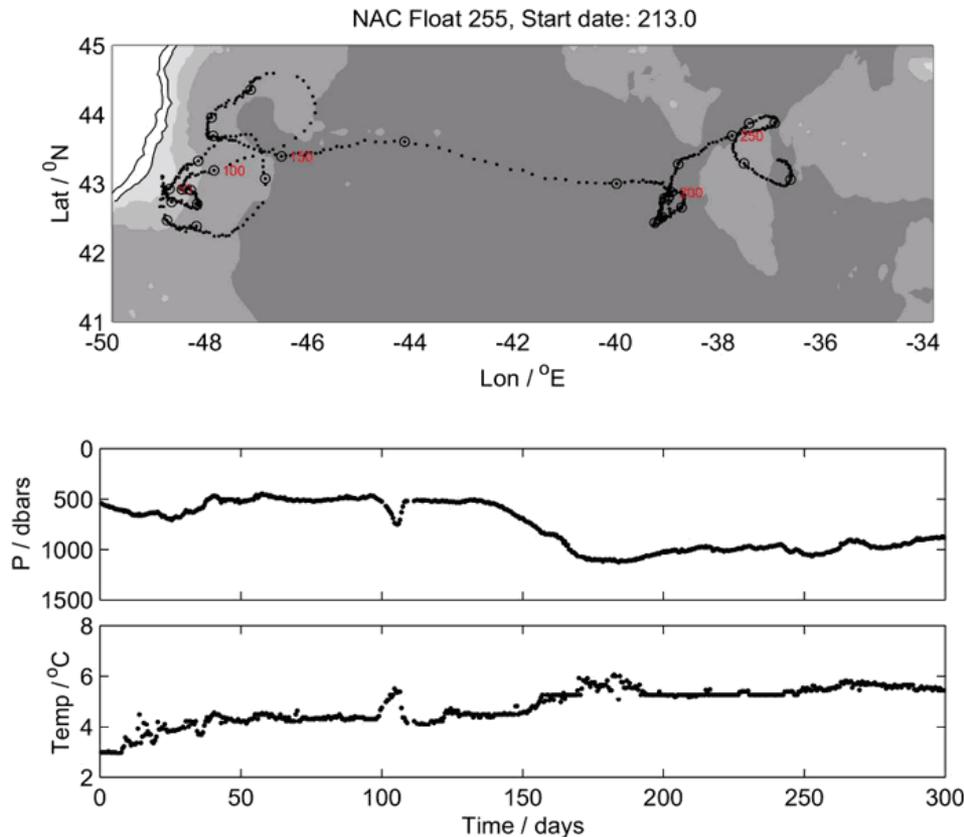


– Mooring data are temporally & vertically ‘continuous’.

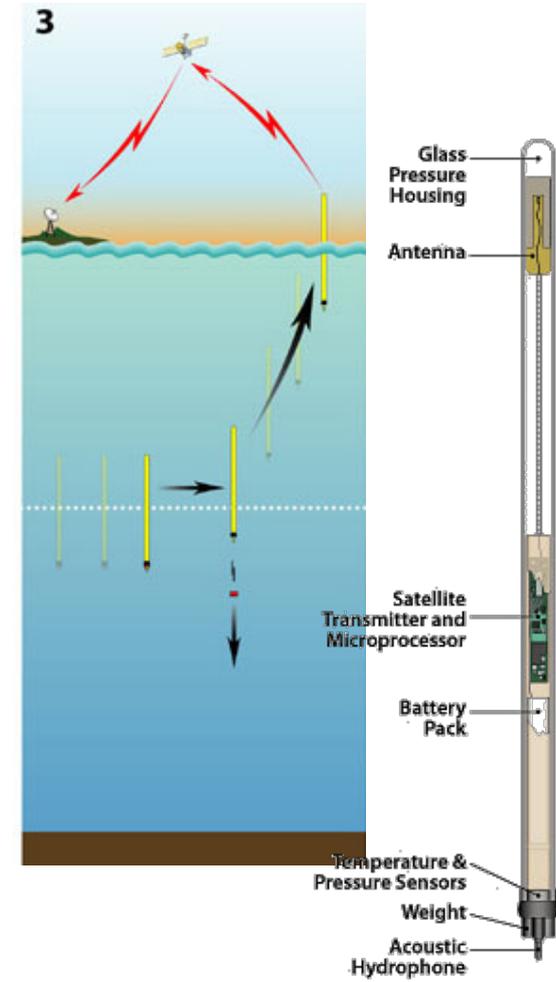
<http://www.pmel.noaa.gov/tao/jsdisplay/>

# In-Situ Instruments(Movable Lagrangian) Platform. Floats

- ◆ Argo Floats. Observation on the isopycnal surface
  - $(T,S)$  by CTD
  - $(u,v)$  derived from positionalong  $(\mathbf{x}^{(2D)})(t_k), p(\mathbf{x}^{(2D)})(t_k))$  in upper 2000m

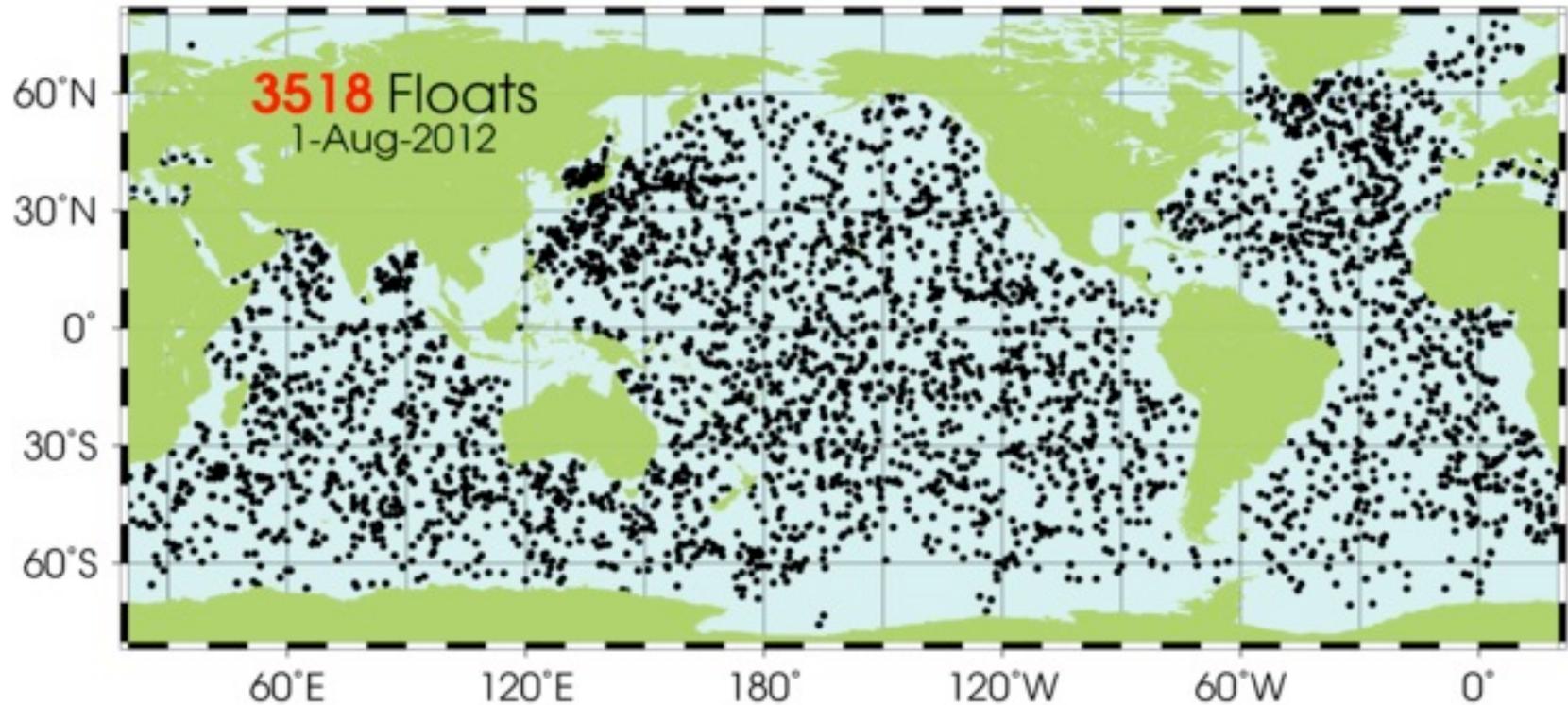


<http://www.dosits.org/gallery/tech/ooc/rafos1.htm>



<http://www.whoi.edu/instruments/>

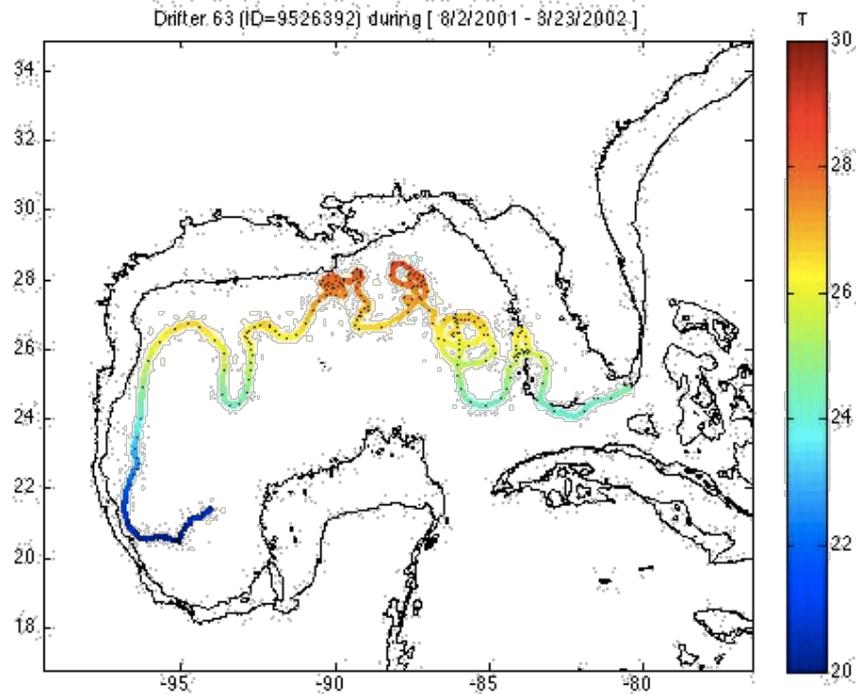
# Global Ocean Observing System by ARGO Floats



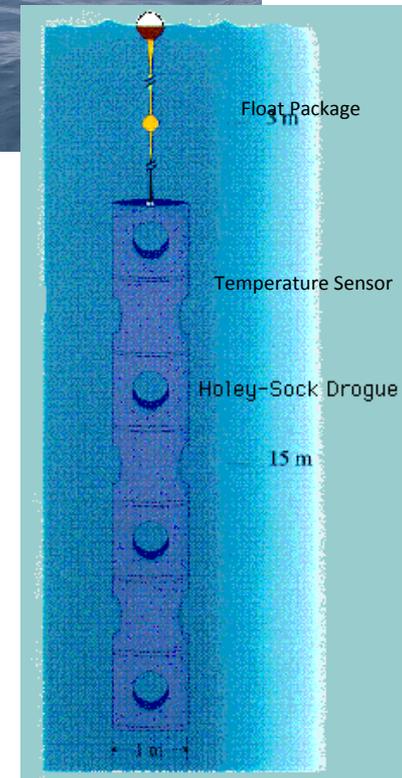
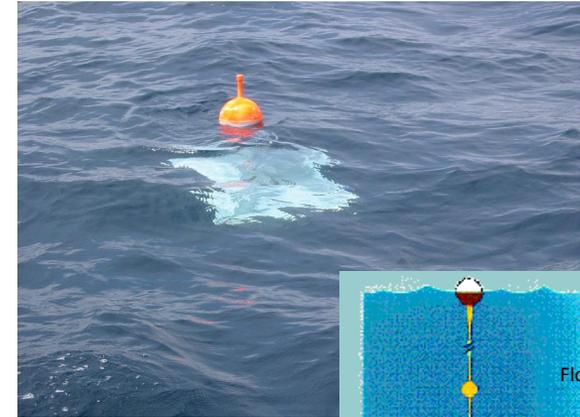
- ▶ Argo are used as the platform for continuous observation
  - ◆ Eulerian observations of  $T$ ,  $S$ , and velocity
- ▶ By November 2007, Global observation network by drifters is 100% complete
  - ◆ ~3000 profiling at the  $5^\circ \times 5^\circ$  resolution
  - ◆ 800 floats per year to maintain the level

# In-Situ Instruments(Movable Lagrangian) Platform. Drifters

- ◆ Observations at sea surface
  - $T$  : Temperature along  $(\mathbf{x}^{(2D)})(t_k)$  at sea surface

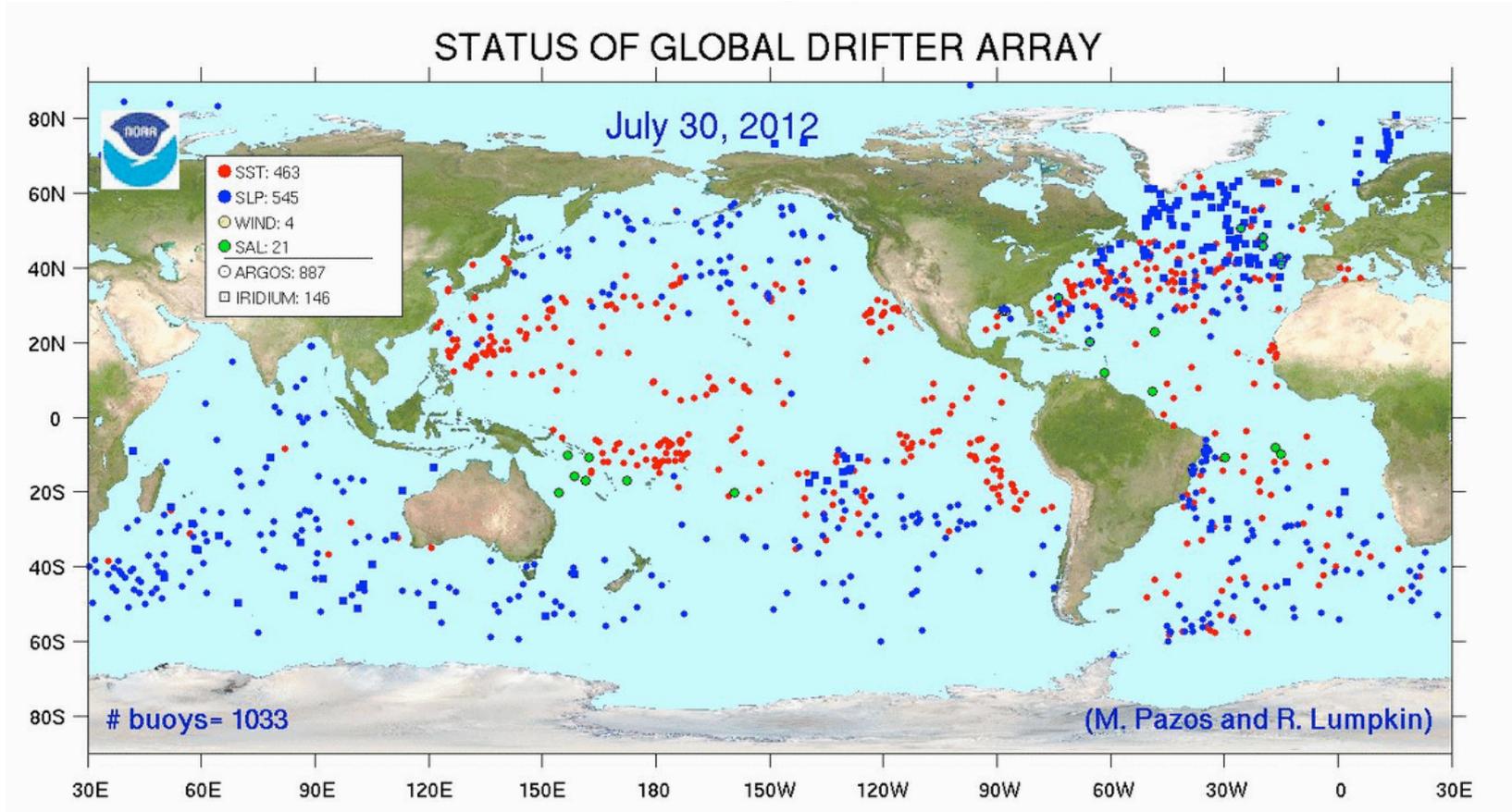


Data available from  
<http://www.aoml.noaa.gov/phod/dac/dacdata.html>



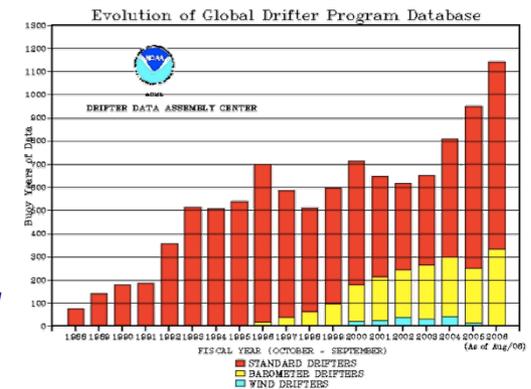
<http://www.drifters.doe.gov/design.html>

# Global Ocean Observing System by Drifters



- ▶ Global observation network by drifters
  - ◆ ~1200 drifters to cover at the  $5^{\circ} \times 5^{\circ}$  resolution
- ▶ Drifters are used as the platform
  - ◆ Eulerian observations of  $T$  (SLP, Wind)

<http://www.aoml.noaa.gov/phod/dac/gdp.html>



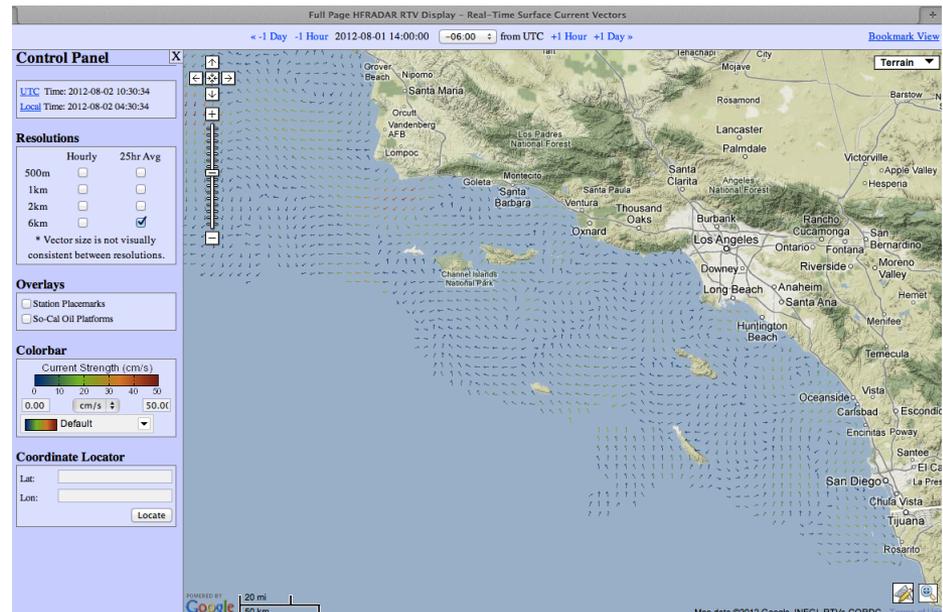
# Remote-Sensing by HF Radar Surface Current

- ◆ Actual measurement: Radial velocity
  - 2 observations makes 2D velocity



<http://www.cocmp.org/>

<http://www.sccoos.org/data/hfrnet/>



# In-Situ Instruments. Vertical Profile

- ◆ BathyThermographs: Temperature recorders.  $\sigma^0_T \sim 0.1-0.2^\circ\text{C}$ 
  - Mechanical (MBTs):
    - Lowered and then winched from the ship down to  $\sim 300\text{m}$ .
  - Expendable (XBTs):
    - Dropped from a ship;
    - Designed to fall at a constant rate..
    - Many goes to 460/760m, some goes to 1800m

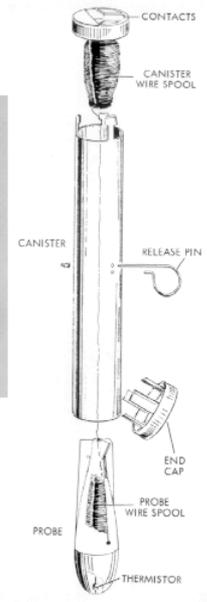
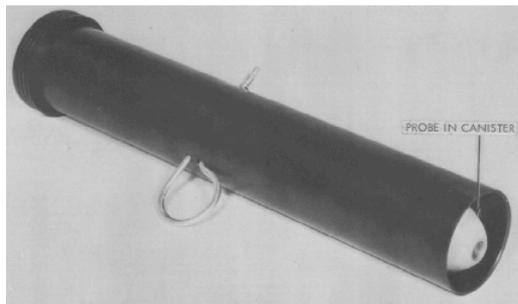
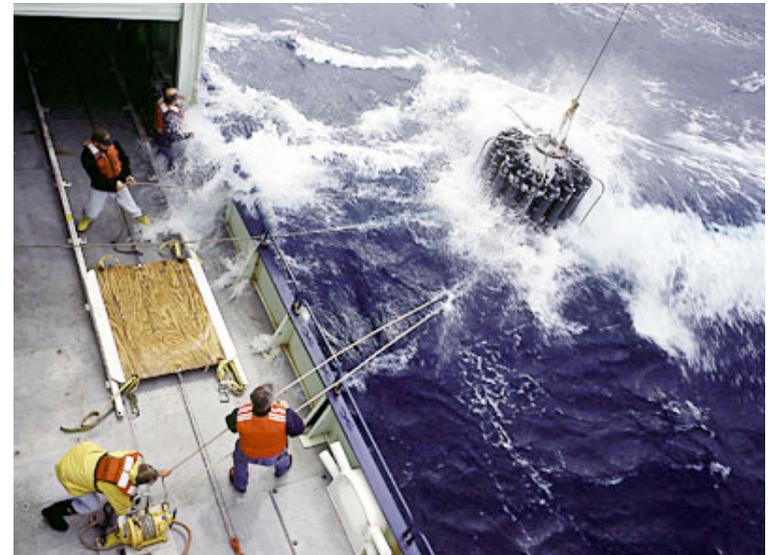


Fig. 1: XBT diagrams: Bathythermograph (probe) and exploded view.



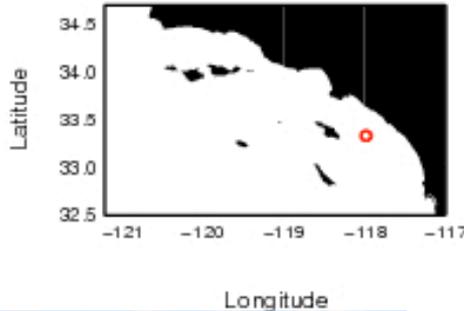
## In-Situ Instruments. Vertical Profile

- ◆ Conductivity, Temperature, & Depth (CTD): High-quality T/S profile of 150 levels ( $\sigma^0_T, \sigma^0_S$ )  $\sim$  (0.002°C, 0.005psu)

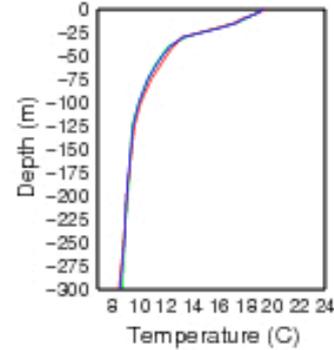


Ship deployed CTD  
Woods Hole Oceanographic Institute

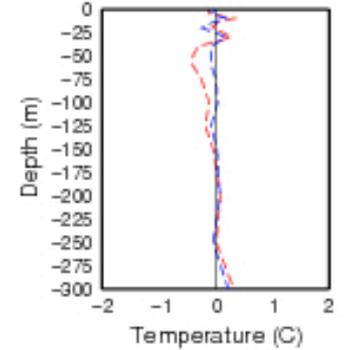
# In Situ Instruments (Movable Platform): Glider



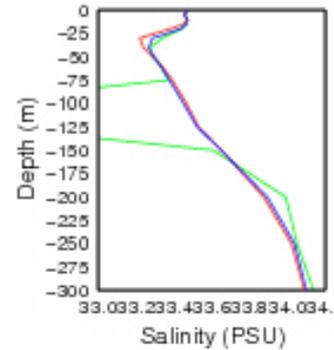
Temperature Profiles



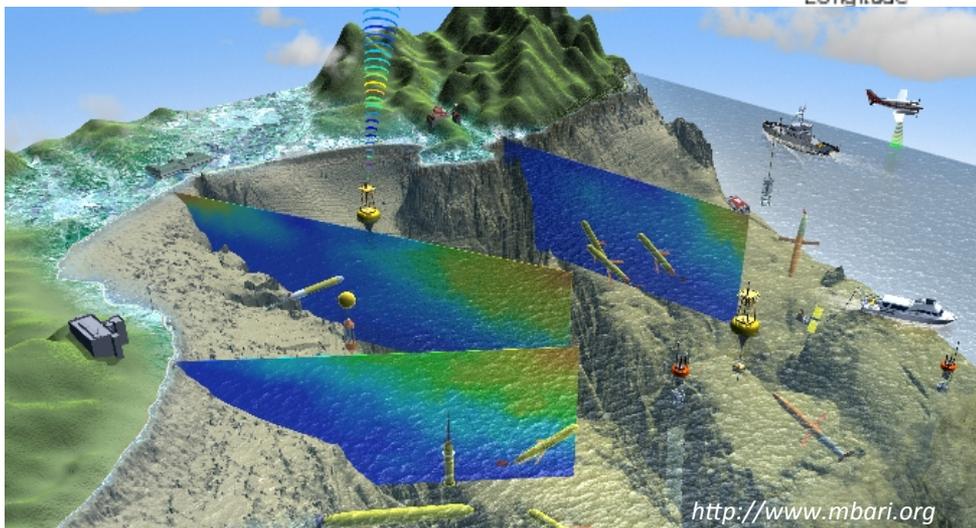
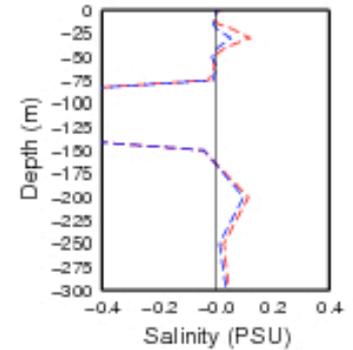
Temperature Difference



Salinity Profiles



Salinity Difference



<http://ocean.jpl.nasa.gov/SCB>

- ◆ Glider
  - 2D position,  $p$  (depth)
  - $T, S$

# Basic Ideas for Ocean Data Quality Control

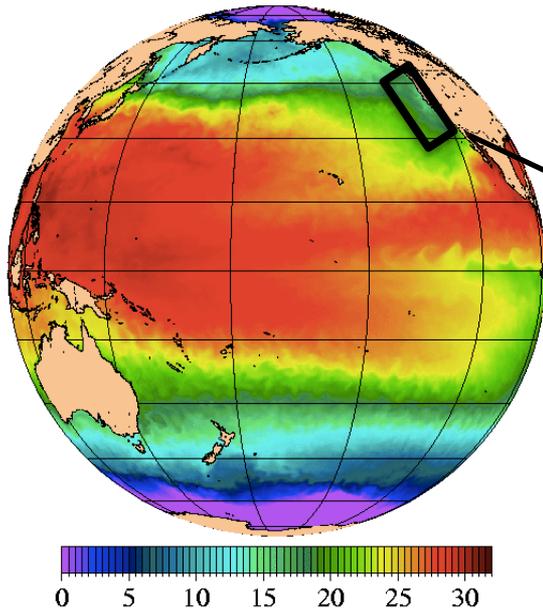
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# Navy Coupled Ocean Data Assimilation

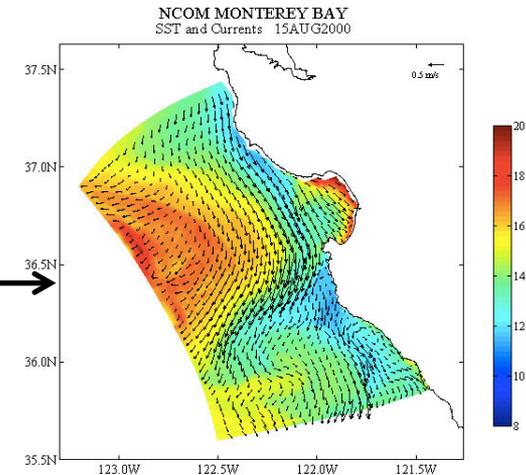
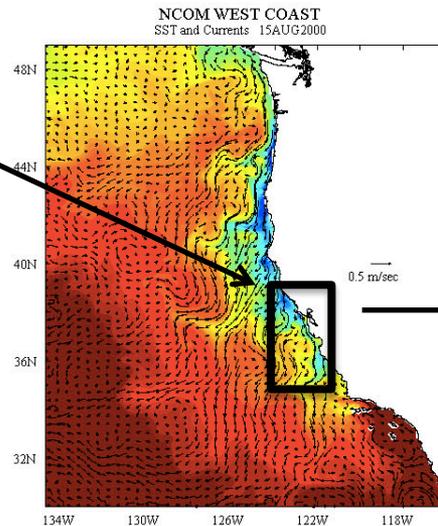
## ◆ Philosophy:

- Approaches to ocean data assimilation vary widely both in terms of the sophistication of the method and the observations assimilated, and also in terms of specification of the forecast error covariances, model biases, observation errors, and quality-control procedures
- Quality Control should be fully automated and performed in stages

Sea Surface Temperature (C)  
NRL global NCOM glb8\_2f  
08-15-2000 00Z 0000 m



Nested & Relocatable

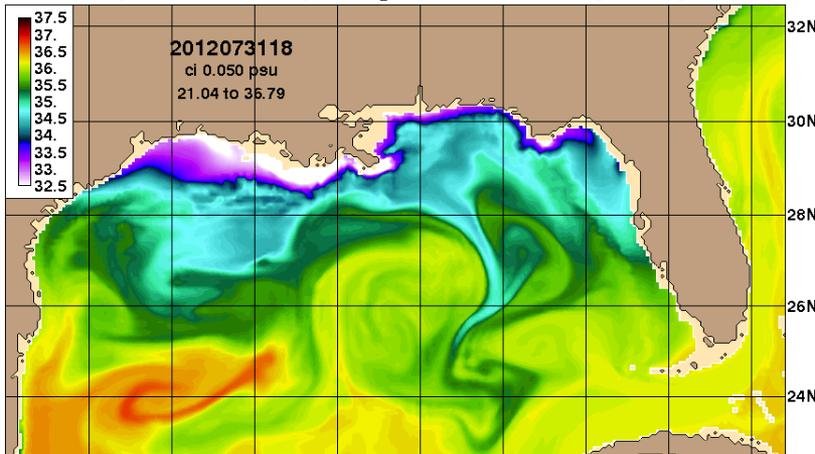




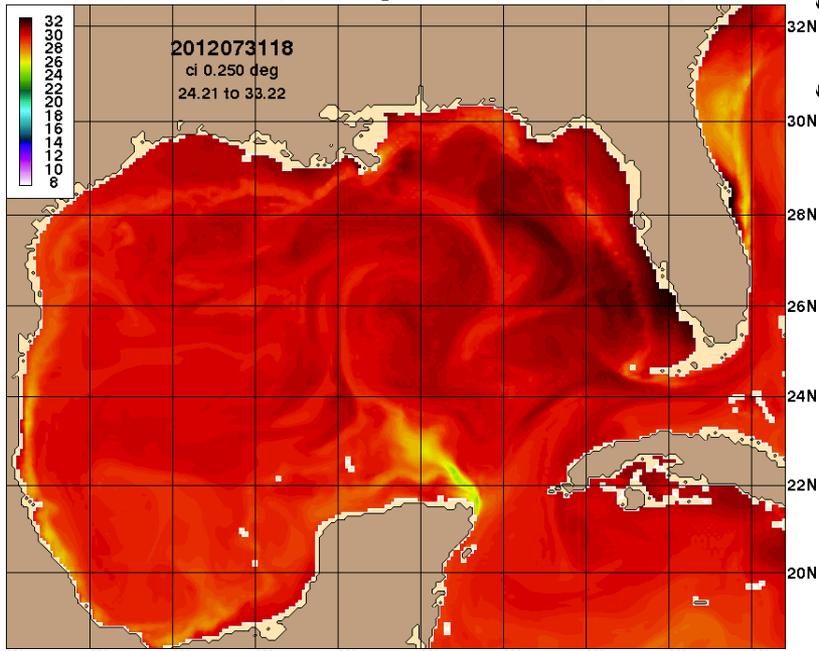
# Navy Coupled Ocean Data Assimilation

## ◆ Real-Time 1/12o Nowcast/forecast system

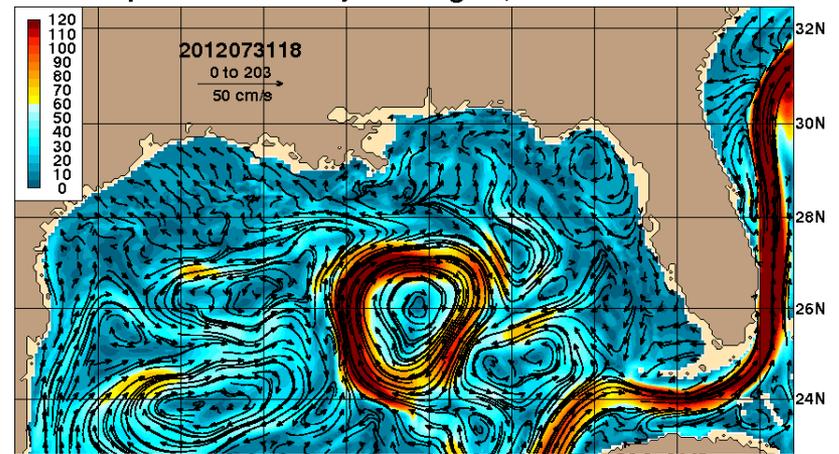
layer=01 salinity Aug 06, 2012 00Z [90.9H]



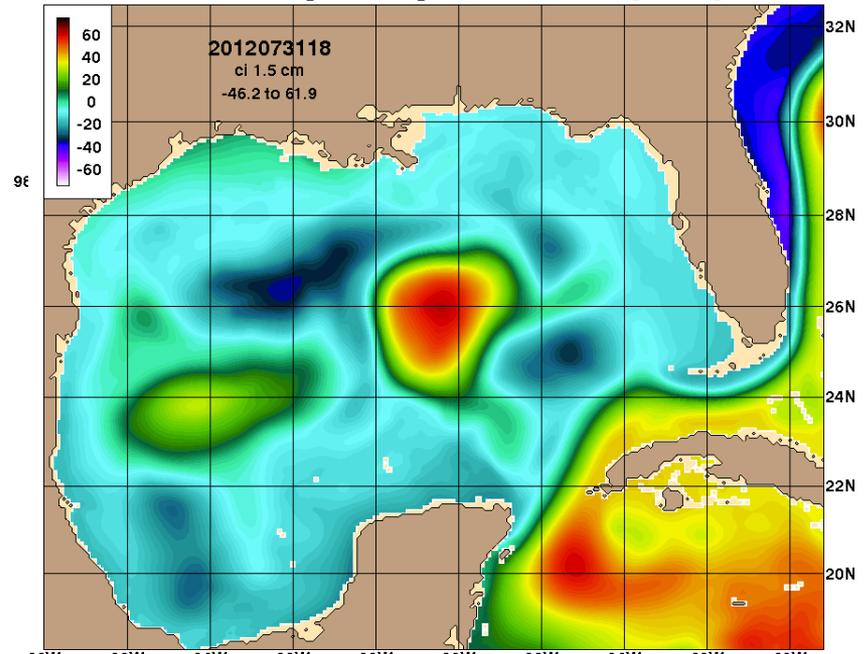
layer=01 temp Aug 06, 2012 00Z [90.9H]



Speed/currents layer 1 Aug 06, 2012 00Z 90.9



sea surf. height Aug 06, 2012 00Z [90.9H]



# Navy Coupled Ocean Data Assimilation

- ◆ Quality Control in 3 Stages according to Ingleby and Huddleston (2007)
  - Stage I. Sensibility Check
    - Land/sea boundary checks
    - Location (speed) test for drifters and ship (aircraft) observations
    - Exact and near-dup duplications

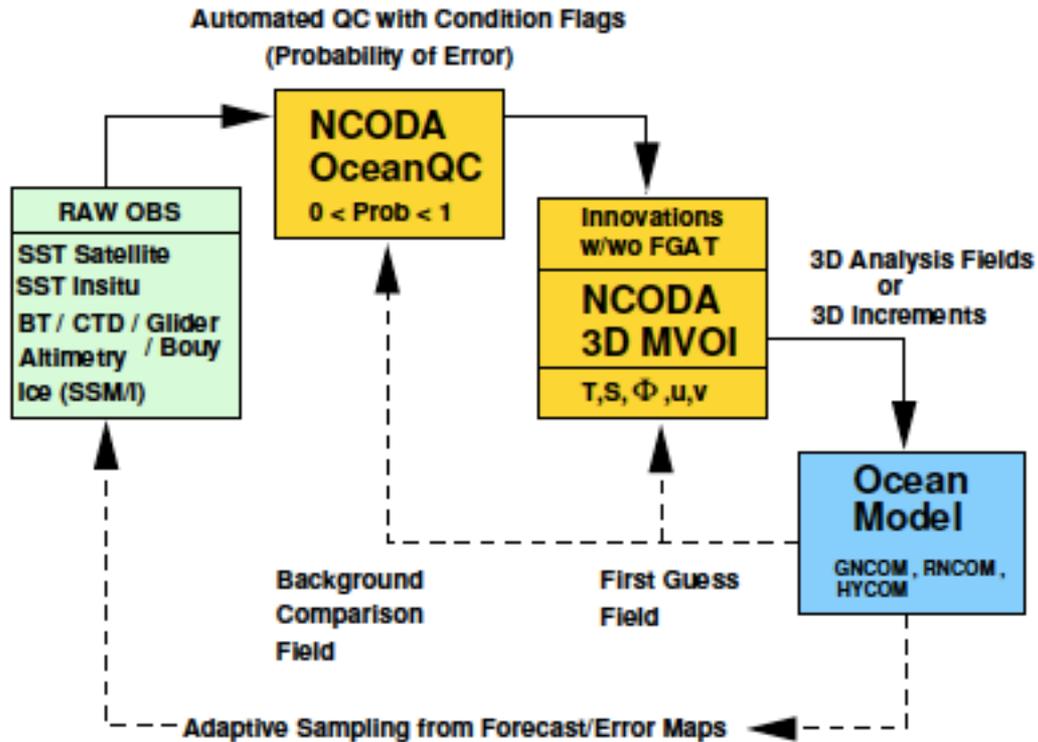
→ *Observations failing sensibility checks are removed*
  - Stage II. Gross error checks
    - Instrumentation error, vertical gradient, static stability checks
    - Cross validation checks (e.g., SST vs sea ice)
    - Background field checks against climate, previous analysis/forecast
    - Bouy (float) sensor drift
    - Satellite SST large scale aerosol/dust bias detection

→ *Observations failing sensibility checks are flagged*

→ *All gross error checks performed before decision to accept/reject*
  - Stage III. Consistency checks
    - Innovation error checks performed within analysis

# Navy Coupled Ocean Data Assimilation

## ◆ NCODA data flow chart

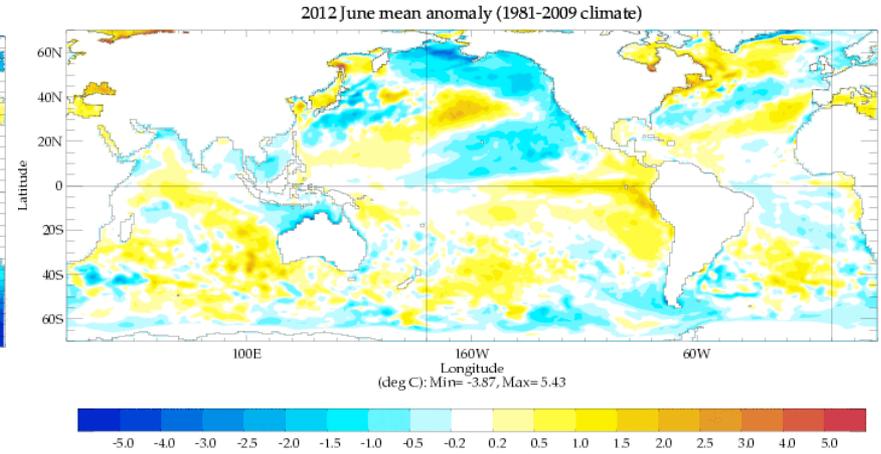
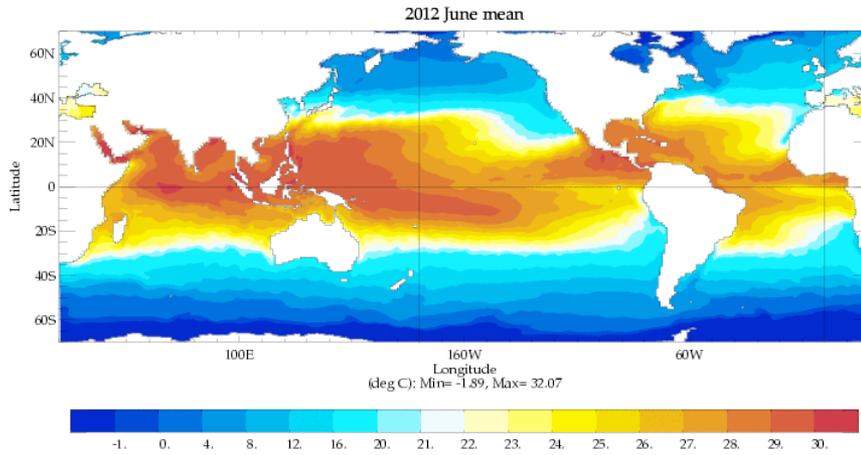


# ECMWF ORA-S4 (Ocean Re-Analysis System 4)

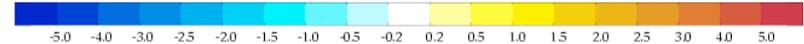
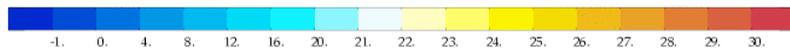
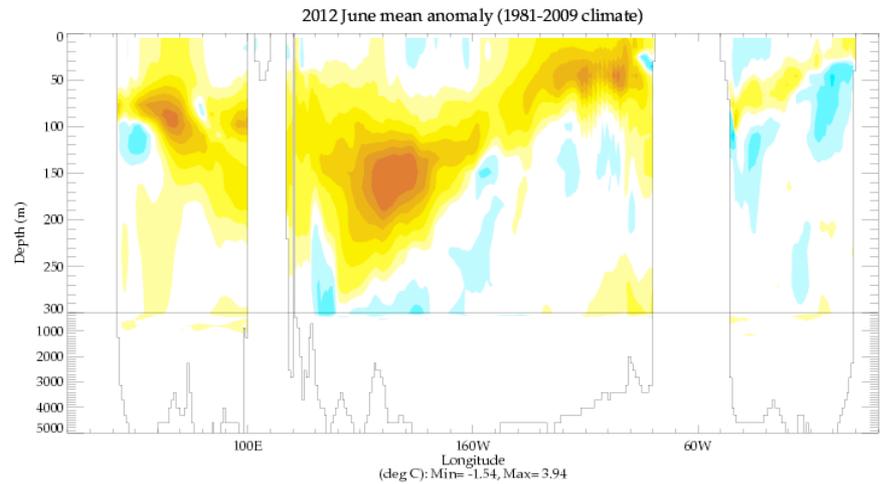
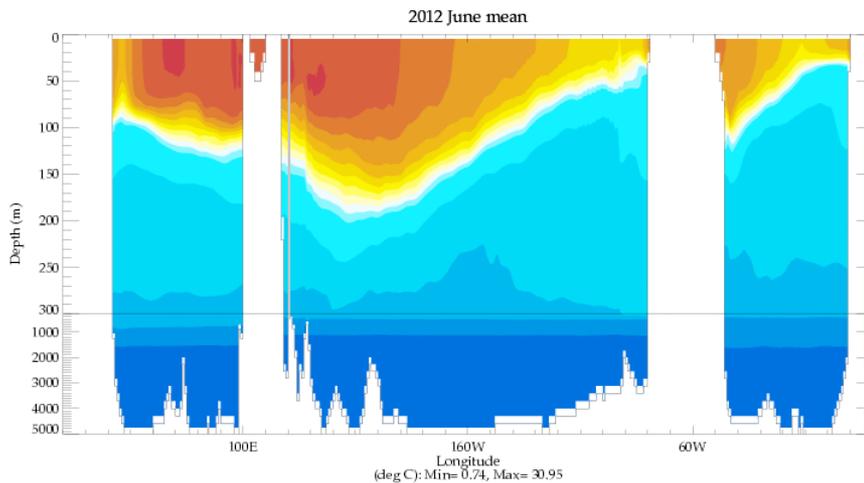
- ◆ Global ocean near real-time analysis & reanalysis since 2012
  - Daily starting from September 1957 & continuously maintained up to 10 days behind real time at 1°x1°x42 level resolution
  - Main purposes: to provide
    - Initial conditions for seasonal/monthly forecasts
    - Historical representation of ocean for climate studies
    - Uncertainty estimates by ensemble (5 total)
  - Featuring
    - Online bias-correction algorithm
    - Assimilation of salinity data
    - Assimilation of altimeter-derived sea level anomalies
  - Designed to reduce spurious climate variability due to observing system change while taking advantages of the new observations
- ◆ Previous systems
  - System 1 (ORA-S1) starting 1997
  - System 2 (ORA-S2) introduced in 2000
  - System 3 (ORA-S3) introduced in 2006

# ORA-S4 : 3D evolution of ocean state

## ◆ Sea Surface Temperature



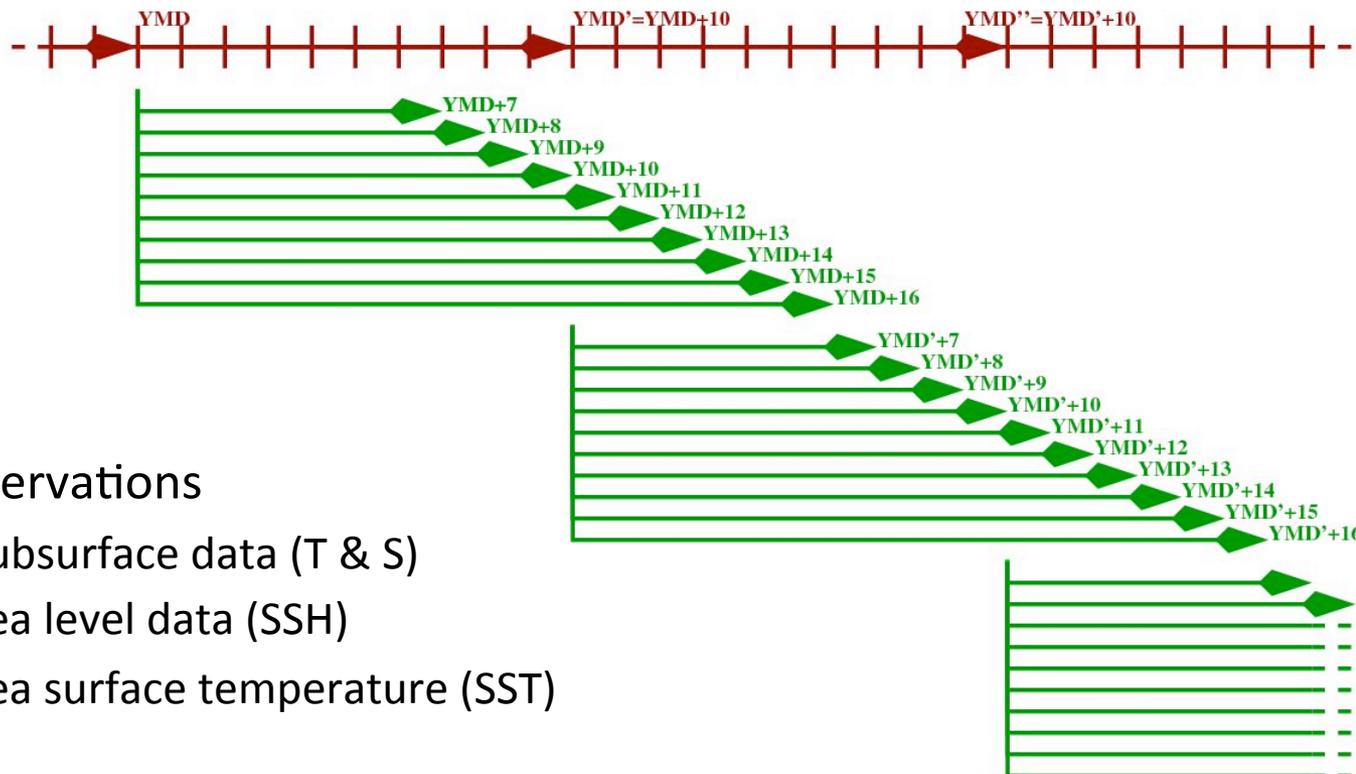
## ◆ Cross-Section at the Equator



# ECMWF ORAS4 & ORTS4 (Ocean Re-Analysis & Real Time )

## ◆ Operational schedule for the production of ORAS4 & ORTS4

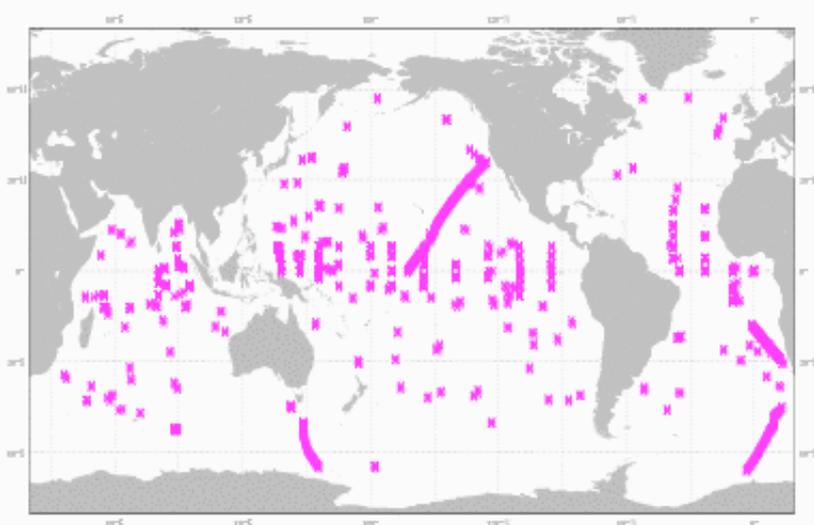
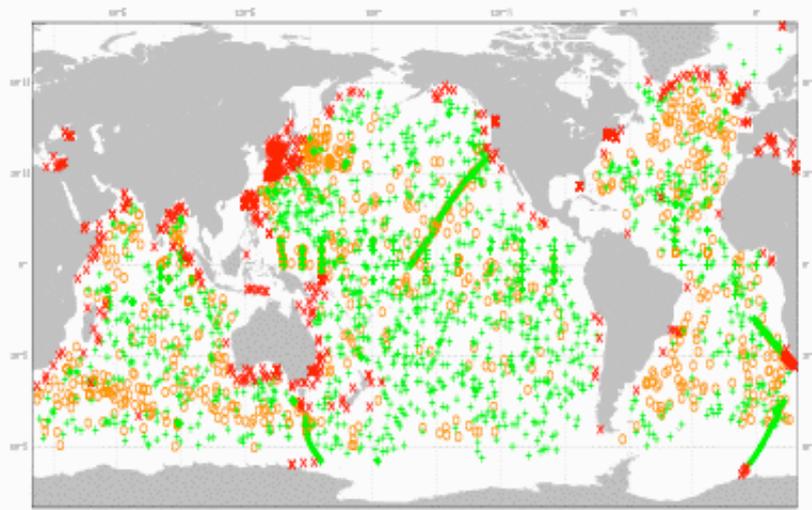
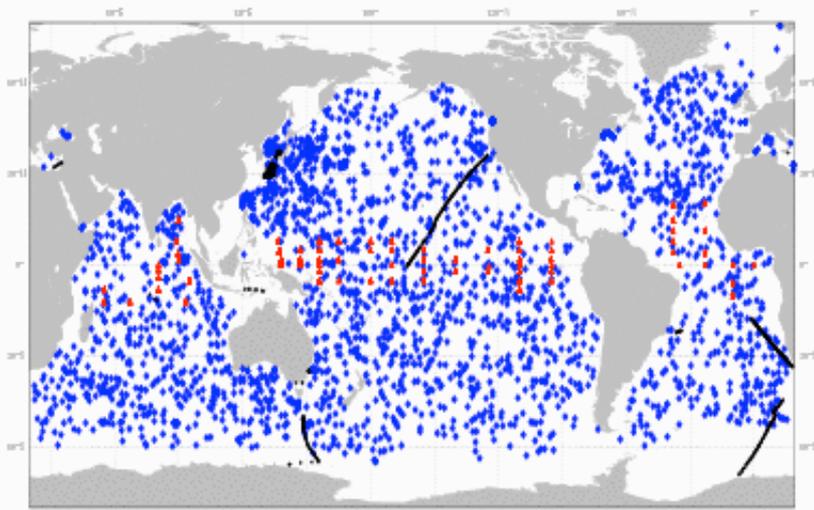
- Reanalysis: every 10 days, with a delay of 6 days to wait for the arrival of ocean observations (in particular, retrieval of the sea-level products)
- Real-time: to create real-time initial condition on a daily basis, ORTS4 brings the latest ORAS4 state up to real time every day, using available observations in a variable assimilation windows



## ◆ Observations

- Subsurface data (T & S)
- Sea level data (SSH)
- Sea surface temperature (SST)

# ECMWF ORAS4 & ORTS4: Data Coverage (Subsurface T)



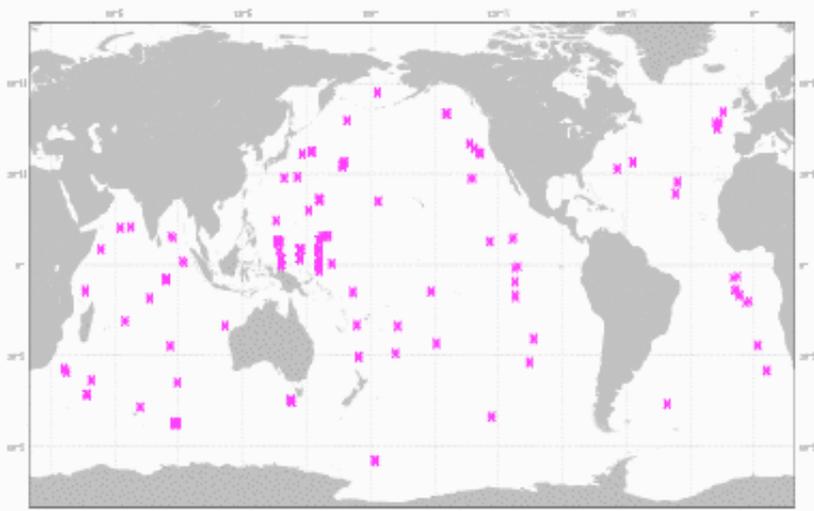
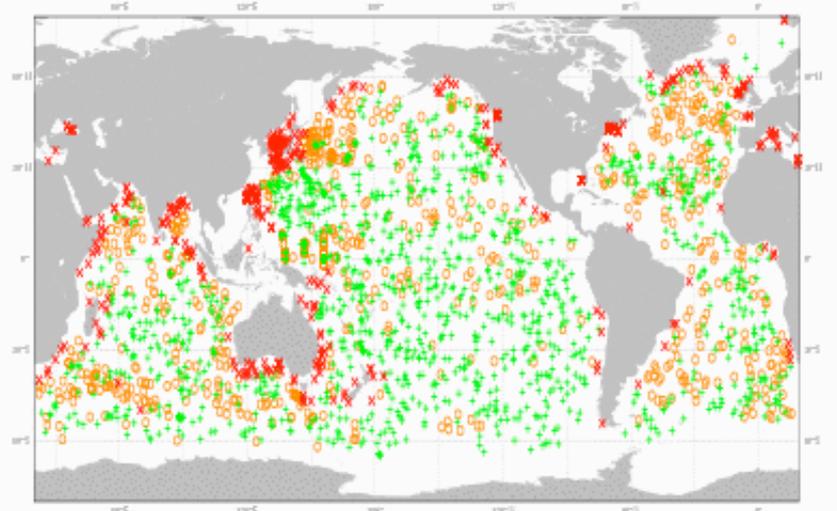
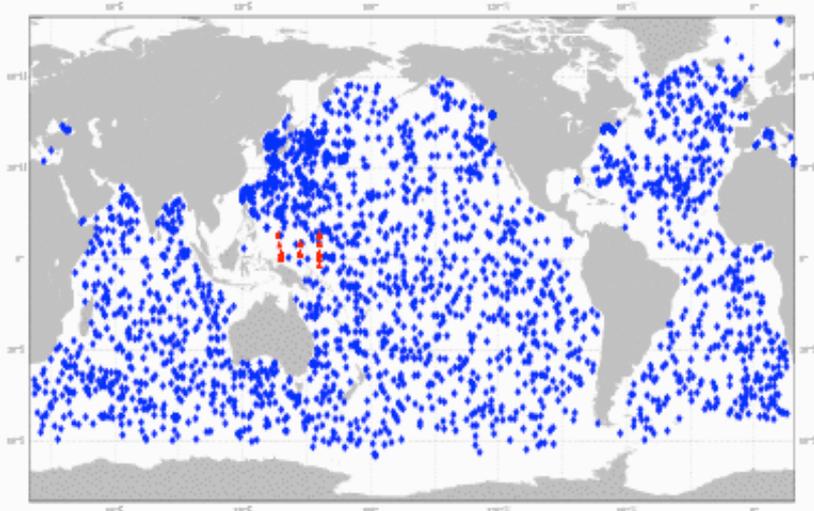
**XBT probes: 500 profiles**  
**Argo floats: 2719 profiles**  
**Moorings: 891 profiles**

**Partially Accepted: 947 profiles**  
**Fully Accepted: 2398 profiles**  
**Fully Rejected: 765 profiles**

**SuperObs: 1566 profiles**  
**(at least one per profile)**

**In situ observation monitoring (temp)**  
**S3 ocean analysis**  
 10 days period centered on 20120225

# ECMWF ORAS4 & ORTS4: Data Coverage (Subsurface T)



**Argo floats: 2578 profiles**  
**Moorings: 169 profiles**

**Partially Accepted: 814 profiles**  
**Fully Accepted: 1356 profiles**  
**Fully Rejected: 577 profiles**

**SuperObs: 360 profiles**  
**(at least one per profile)**

**In situ observation**  
**monitoring (sal)**  
**S3 ocean analysis**  
10 days period centered on 20120225

# Ocean Observation and Quality Control for ORA & ORT-S4

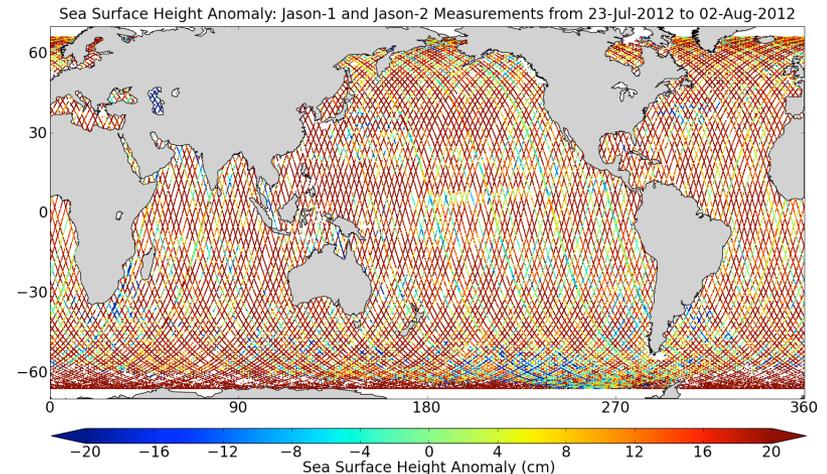
## ◆ Automatic Quality Control for subsurface data

1. *Daily averaging.* If some site reports more frequently than once per day, daily averages are created.
2. *Blacklist of coastal observations.* Data in the vicinity of the coast are rejected, as a way of accounting for representativeness error.
3. *Background check.* A level-by-level check between the distance between model values and observations in relation to the error statistics.
4. *Buddy check.* A consistency test between observations is performed.
5. *Super-obbing.* Profiles which are close in space and time are superobbed
6. *Completeness of profiles.* A profile is considered incomplete, and therefore rejected, if the sparsity of the remaining observations in the vertical is judged insufficient to resolve the vertical temperature gradients. (Ex: An observation profile will be rejected if the temperature difference between consecutive levels is larger than 5 deg C or if it contains a vertical temperature gradient larger than 0.1 deg C/m).

Extension of Smith N., J Blomley, and G Meyers, Prog in Oceanography,1990.

# Satellite Data Quality Control at ECMWF

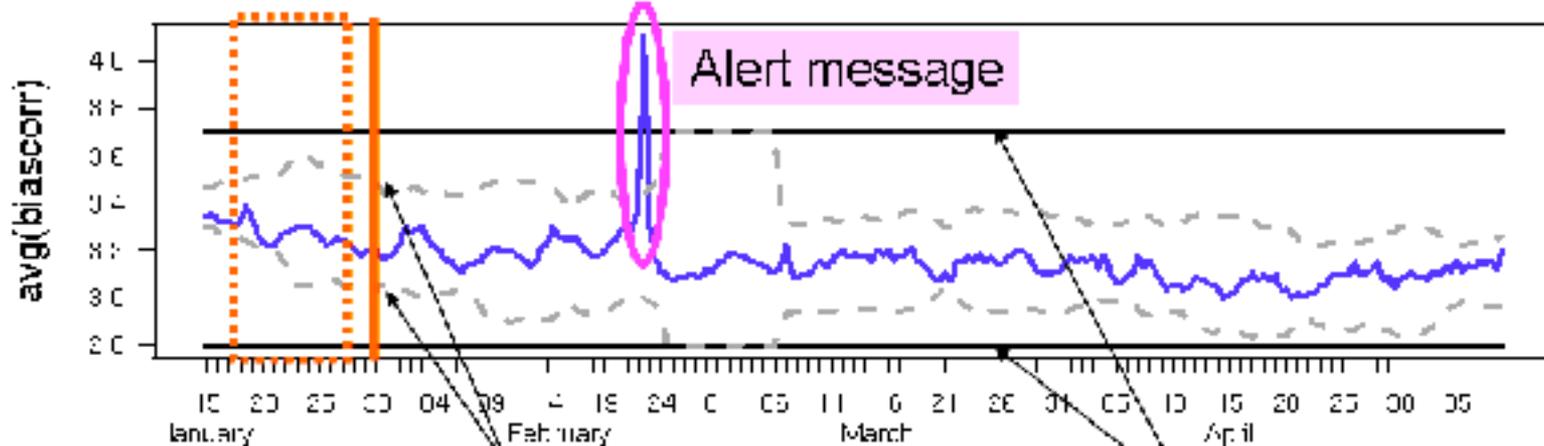
- ◆ Automatic checking – Experimental
  - Recently implemented at ECMWF
  - It triggers alarm messages if an anomaly is detected in the quality or the availability of the satellite data assimilated by the model.
  - Selected statistical parameters
    - number of observations
    - bias correction
    - mean bias-corrected background and analysis departuresare checked against an expected range.
  - Currently, the automatic checking is limited to data passing through the minimization process.



# Satellite Data Quality Control at ECMWF

## ◆ Procedure

- An appropriate alert message (including a time series plot) is generated if statistics are outside the specified ranges.
- A severity level (slight, considerable, severe) is assigned to each message depending on how far statistics are from the expected values.
- Two kinds of ranges are used by the automatic checking:
  - Soft limits are updated automatically using statistics from the last twenty days
  - Hard limits are adjusted manually when required.



Soft limits (mean  $\pm$  5 stdev of statistic to be checked, calculated from past statistics over a period of 20 days, ending 2 days earlier)

Hard limits (fixed)

# Satellite Data Quali

## ◆ Operational Checking

### AIRS

**AQUA AIRS 2097 clear radiances :**

(6 times in last 10 days for

[airs 784 11 2097 210.png](#)

Slightly: avg(biascorr)

**AQUA AIRS 2098 clear radiances :**

(7 times in last 10 days for

[airs 784 11 2098 210.png](#)

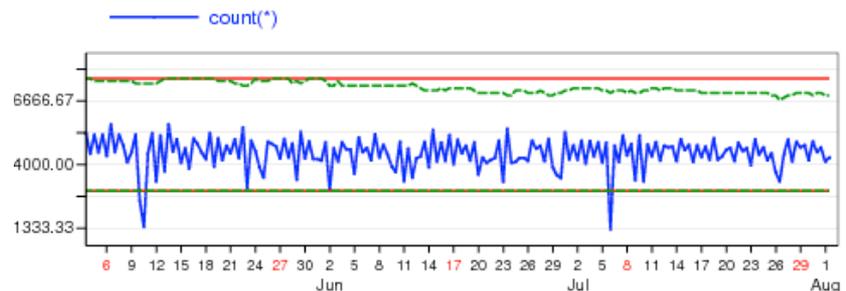
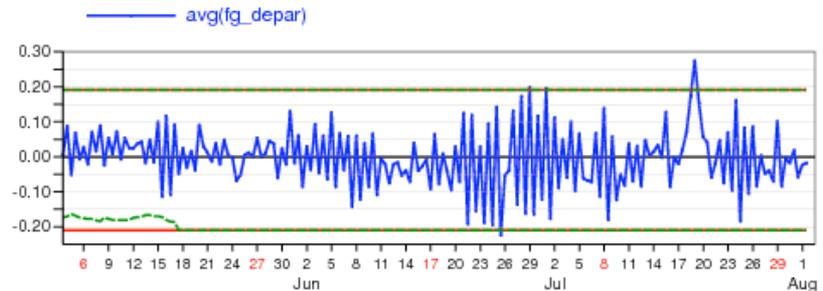
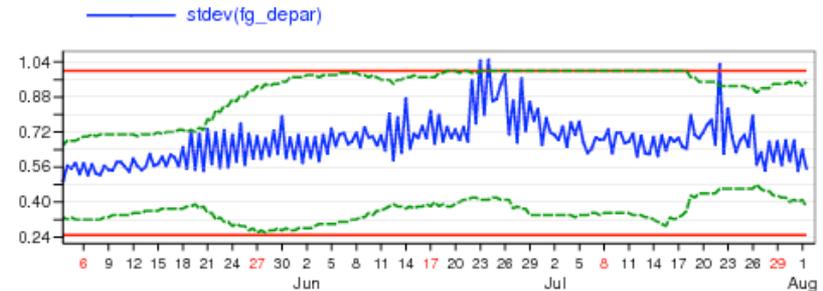
Slightly: avg(biascorr)

**AQUA AIRS 1119 clear radiances :**

AQUA AIRS 2097 clear radiances

Active data, EXP =0001

airs\_784\_11\_2097\_210



# ROMS (Regional Ocean Modeling System) 3D-Var

## ◆ Regional Ocean Modeling System (ROMS)

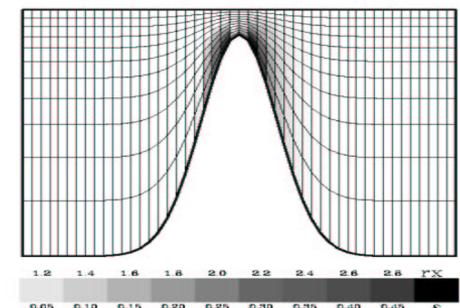
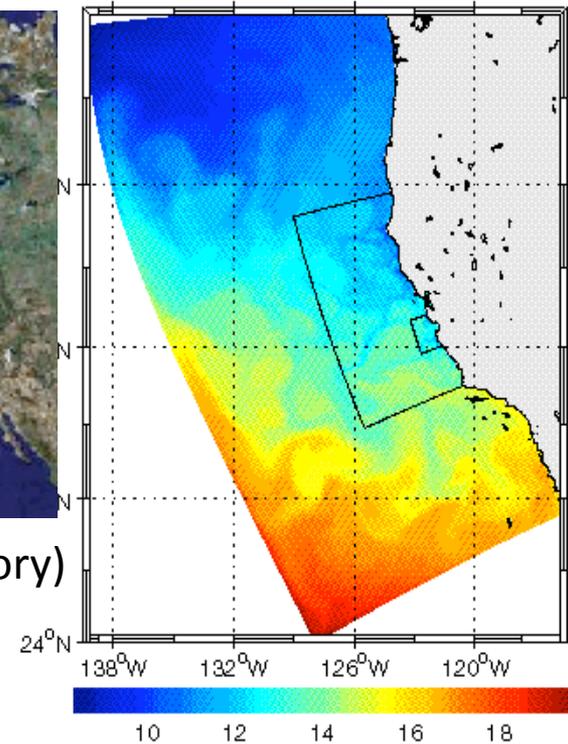
- One-way nested configuration
  - Pacific basin for largest domain
  - Nested coastal configuration
    - » 15km-5km-1.5km-0.5km
    - » Vertical levels >24

– Relocatable, in the future

– Forcing by COAMPS

(Coupled Ocean/Atmosphere

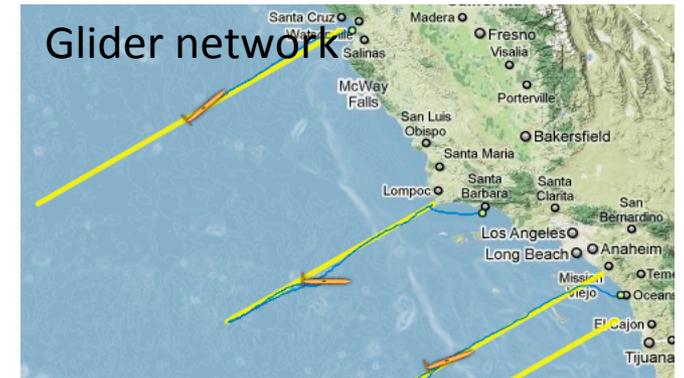
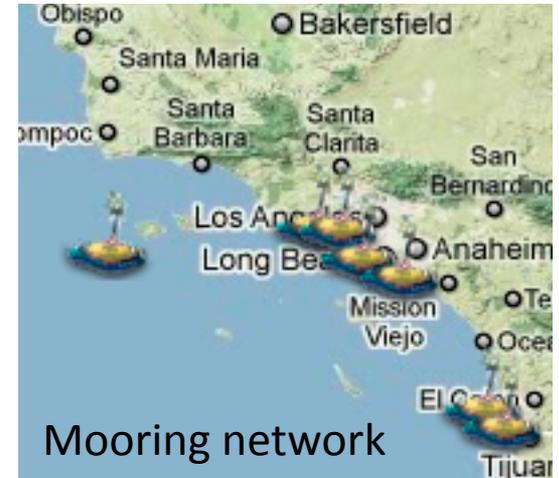
Mesoscale Prediction System by Naval Research Laboratory)



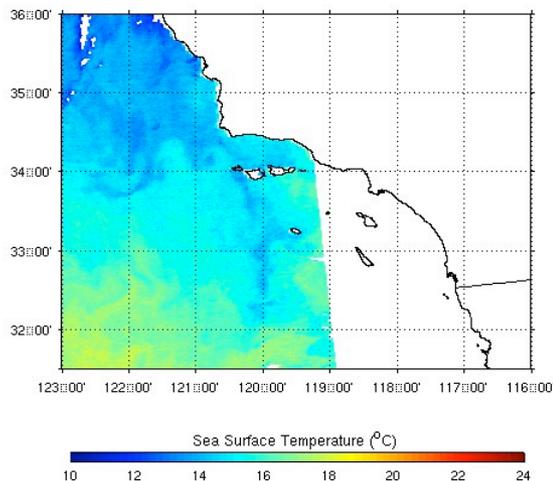
<http://ocean.jpl.nasa.gov/>

# Costal Ocean Observation Network

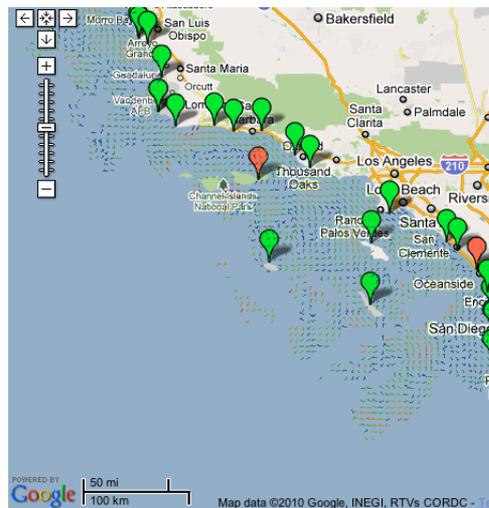
- ◆ Spatial distribution of observing network is highly inhomogeneous
  - Satellite images (SST) can be as high-resolution as the model state in horizontal
  - HR radar (surface velocity) can be highly concentrated and high-resolution
  - Others can be extremely sparse



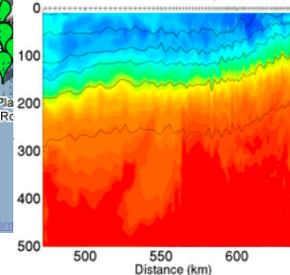
SST on a lucky day



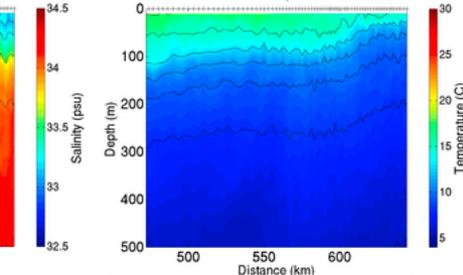
HR radar network



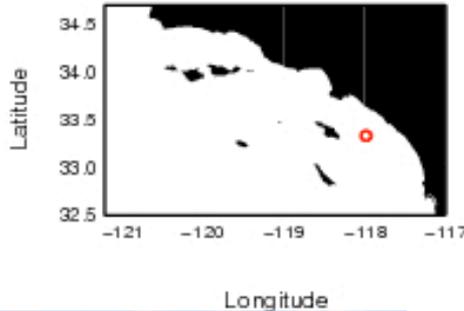
Mission 0030act Salinity, section 2



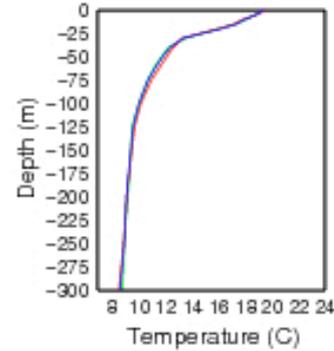
Mission 0030act Temperature, section 2



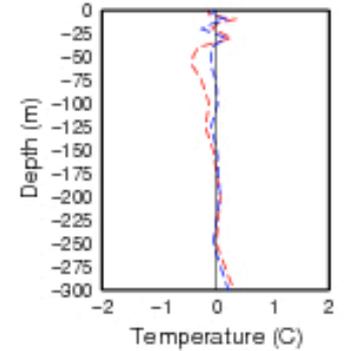
# In Situ Instruments (Movable Platform): Glider



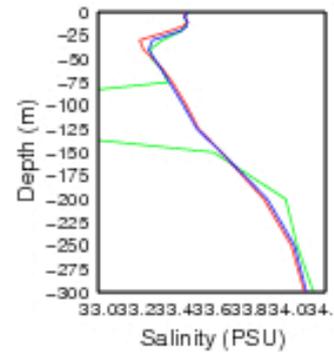
Temperature Profiles



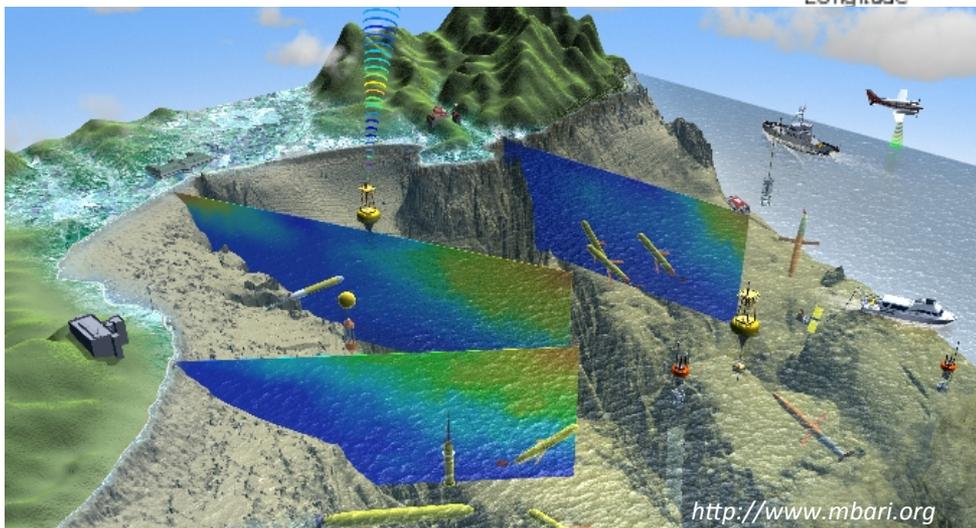
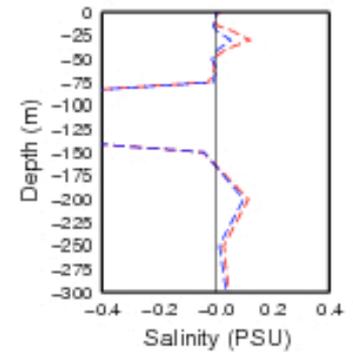
Temperature Difference



Salinity Profiles



Salinity Difference



<http://ocean.jpl.nasa.gov/SCB>

- ◆ Glider
  - 2D position,  $p$  (depth)
  - $T, S$

# Quality Control of In-Situ T/S

- ◆ Developed by Ingleby & Huddleston (2007) at UKMO
- ◆ Principles for building the QC system
  - The system has to be automated to cope with the data volume involved
  - Original, reported values should be used as long as possible (flagged, rather than rejected)
  - Any decisions taken by the system should be traceable
  - The system is designed to support data assimilation
  - Tools to monitor system performance and individual cases are available
  - The generic checks and processing use code shared the UKMO atmospheric QC
  - The generic checks have a clear theoretical basis in probability theory
- ◆ QC Main Steps
  - Data specific check
  - Background and buddy check

## Pre-QC for XBT

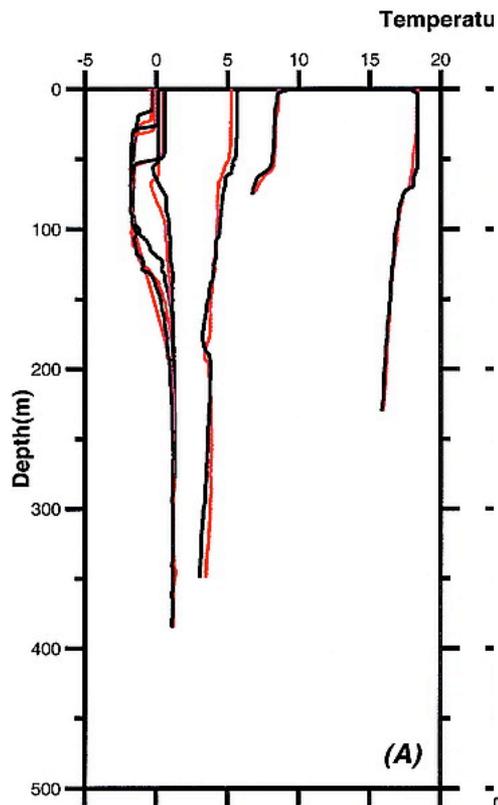
- ◆ Prior rejects for XBT below 1000m due to inaccuracy of the instruments.
- ◆ XBT depth correction: XBT depth is computed based on the time of the release.
  - All XBTs are designed to fall at the known rate, according to the manufacturer's design (formula, or equation for depth vs time from the release).
  - Many won't; revised equation (linear correction) is suggested by Hanawa et al (1995).
  - Depth for the profiles taken before Hanawa et al (1995) were corrected.
  - Additional difficulties:
    - Older data may not have record for type of XBT used
    - In the cold sea, viscosity is higher & drop rate changes.



validated against

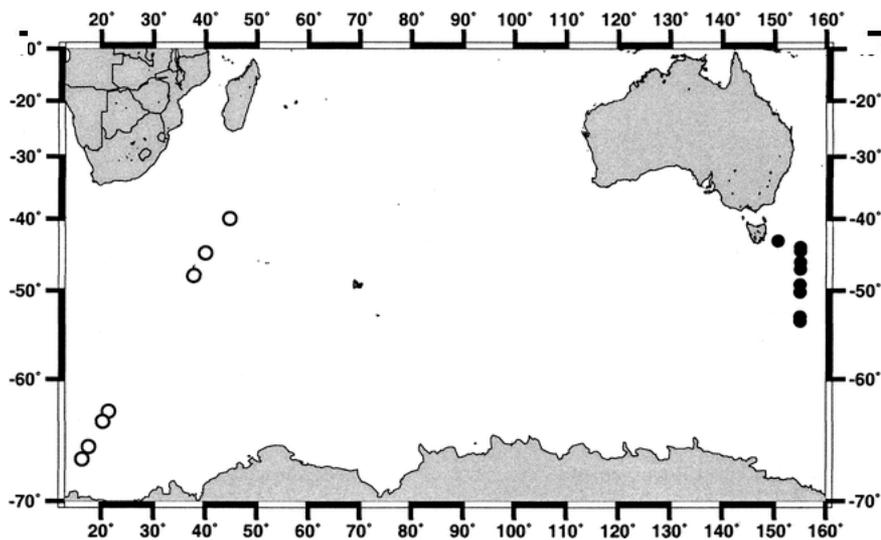
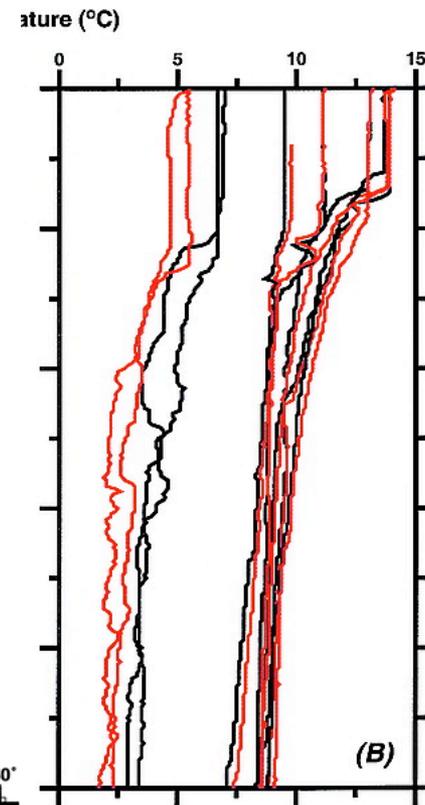


# In Situ Data: XBT vs CTD



Composite profiles of

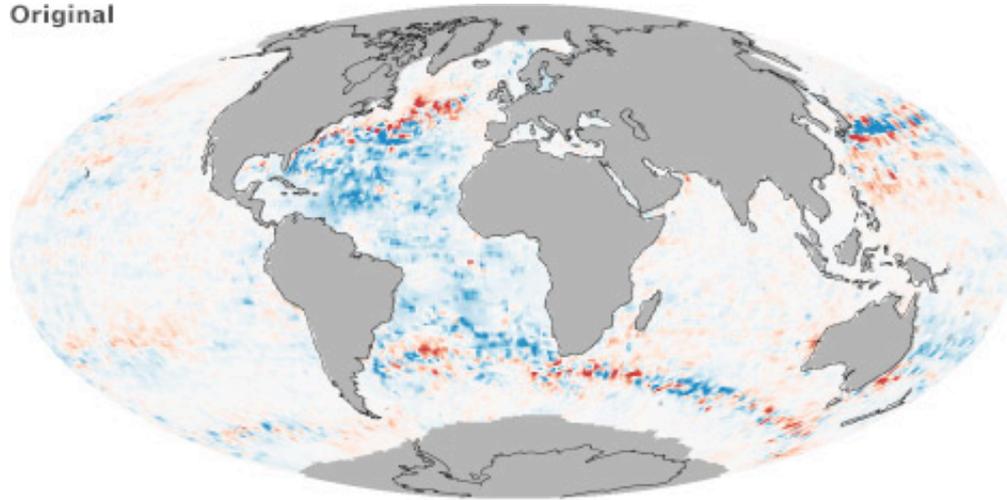
- XBT (red line) and
- CTD (black line)



# Importance of QC / Bias Correction

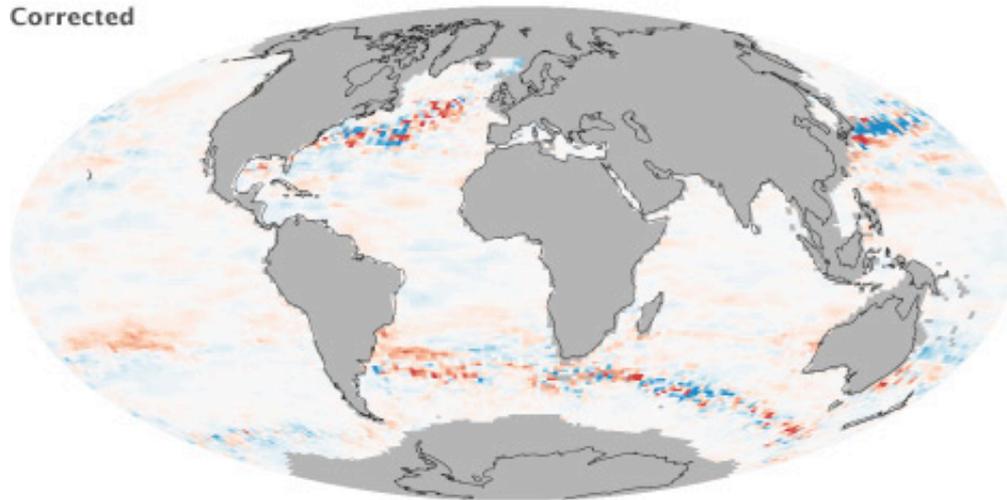
## ◆ Ocean temperature change from 2004 to 2006

Original



Correction in temperature due to bad data from the Argo floats and XBTs

Corrected



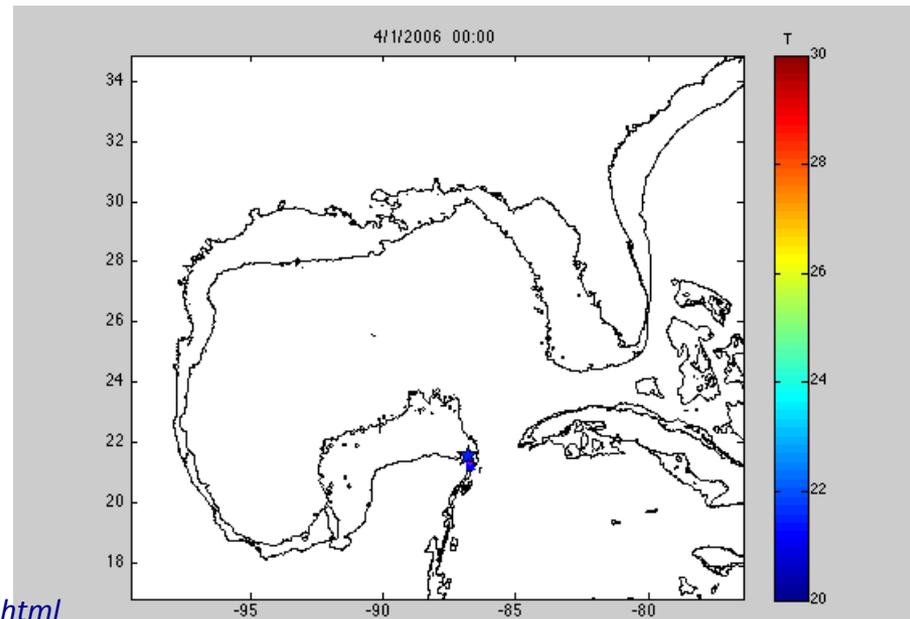
## QC for Data Specific Check

- ◆ Movable instruments
  - Vertical check for the value of data: against constant, spike or step.
  - Horizontal position of the data along the track for each identifier: kinks or jumps.
- ◆ Superobs for mooring in time: TRITON are quasi-hourly but formed into daily averages.
- ◆ Stability check for T/S based on the density for vertical profiles.
- ◆ Duplicate check and thinning in space.

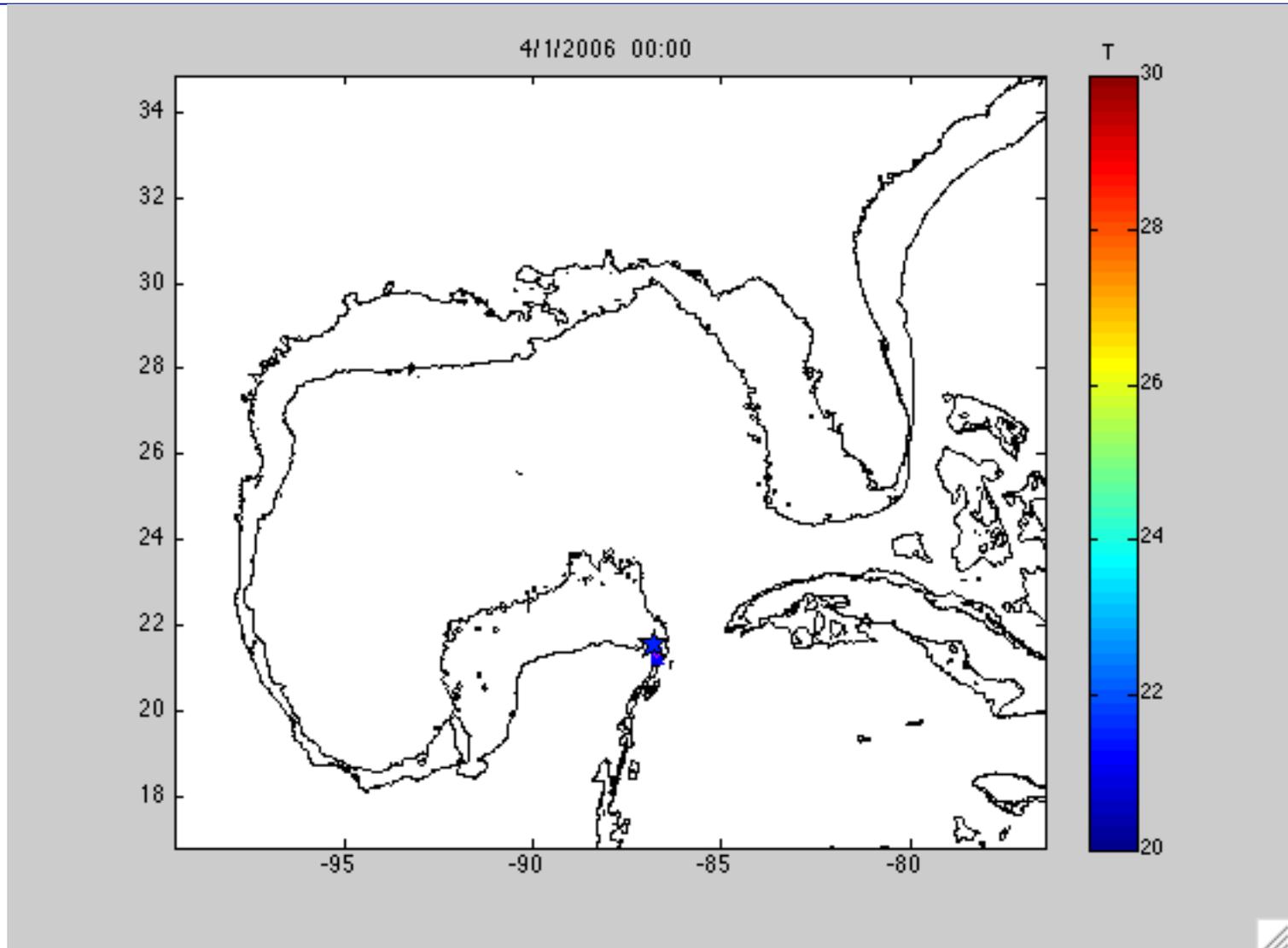
*Background and Observation Buddy Checks are Similar to Atmos QC*

# New Types of Observations

- ◆ Ocean observations are (with respect to atmospheric observations)
    - Sporadic
    - Inhomogeneous
    - Limited to upper ocean
  - ◆ New types of observations that are promising & challenging
    - HF radar observations
    - Lagrangian observations (Position observations along the trajectory)
      - Drifters
      - Floats
      - Gliders (Lagrangian-like)
- with Targeting in mind

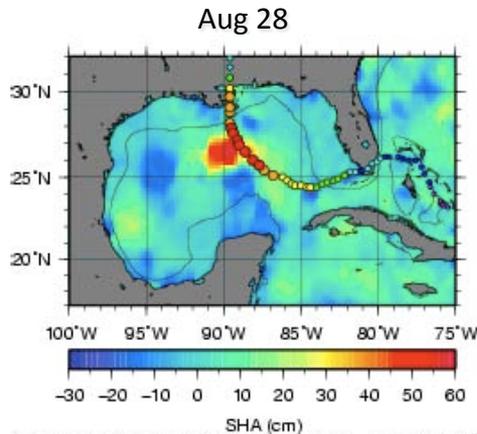


# Lagrangian Data

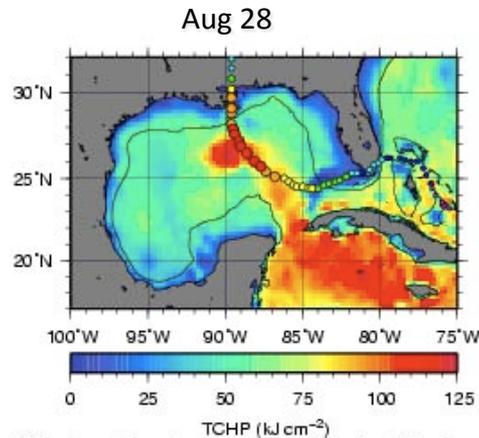


Data available from <http://www.aoml.noaa.gov/phod/dac/dacdata.html>

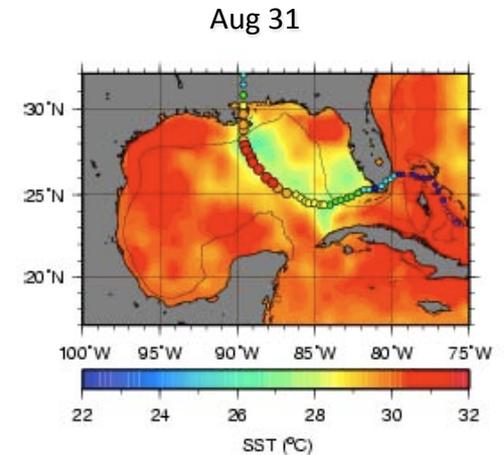
# Additional Motivation: Hurricane Prediction



Satellite altimetry-derived field of sea height anomaly (SHA) on August 28, 2005, in the Gulf of Mexico. The large values (red) of SHA in the center of the Gulf are indicative of the presence of a warm anticyclonic ring. The circles of different colors indicate the track and intensity of Hurricane Katrina. The isobath of 200m is superimposed.



Altimeter-derived estimates of Tropical Cyclone Heat Potential (TCHP) for August 28, 2005. The Loop Current and a large warm anticyclonic ring have the largest amount of heat stored in the region. The circles of different colors indicate the track and intensity of Hurricane Katrina. The isobath of 200m is superimposed.



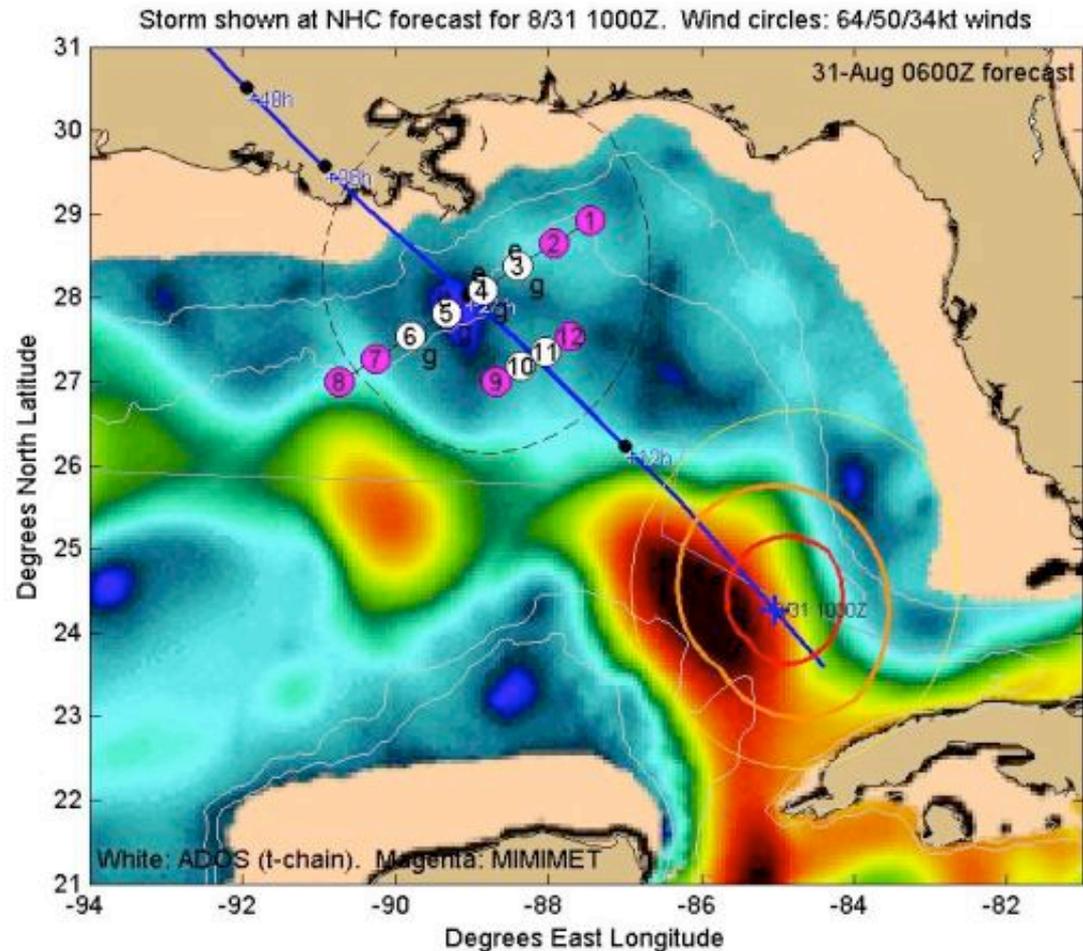
NOAA GOM surface dynamics report for Katrina

<http://www.aoml.noaa.gov/phod/altimetry/katrina1.pdf>

# Adaptive Sampling by Drifters for Better Hurricane Prediction. 1

## ◆ Hurricane Gustav

- 12 drifters deployed in the forecast path of Gustav on August 31, 2008
- All survived and transmitted data

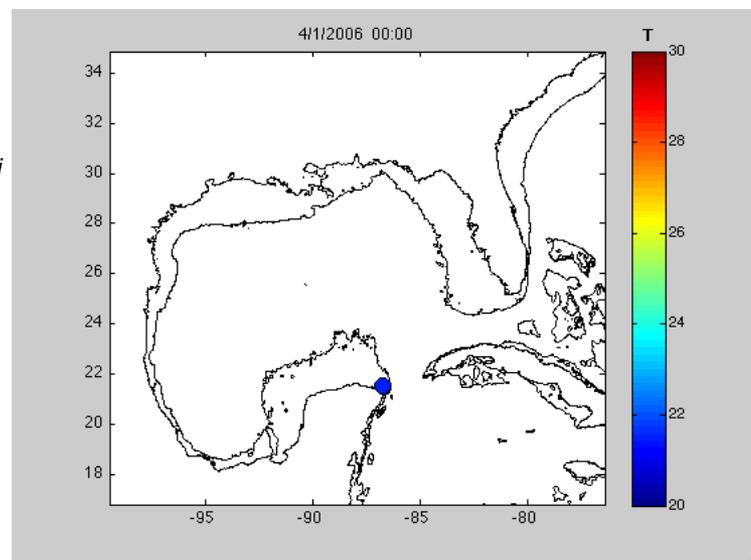
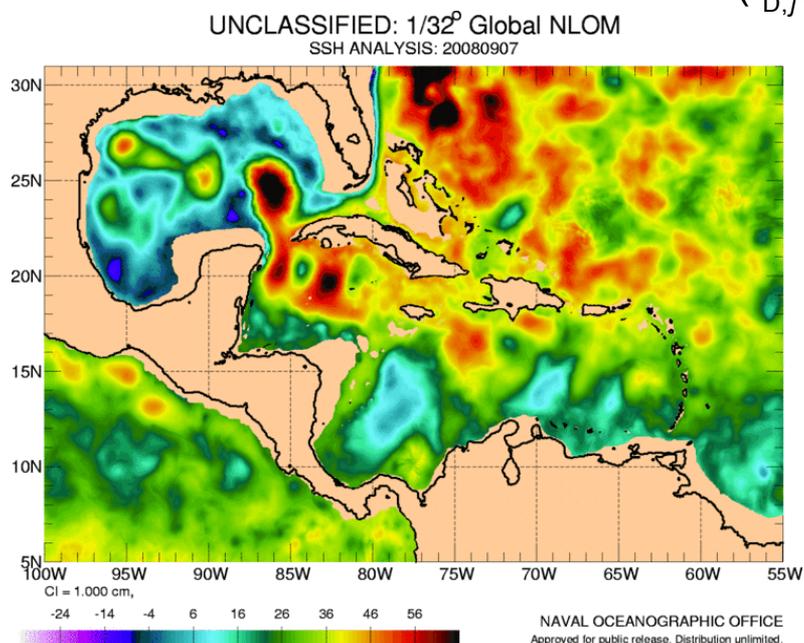


# Ocean Flow and Lagrangian Dynamics

- ◆ Data assimilation attempts to estimate and forecast the evolution of the system (ocean)
- ◆ Ocean flow drives Lagrangian dynamics (drifter motion)
- ◆ How do we do LaDA? Is it effective for estimation and prediction of the flow evolution?

[http://www7320.nrlssc.navy.mil/global\\_nlom32/navo/IAS\\_nlomw12912mooper.gif](http://www7320.nrlssc.navy.mil/global_nlom32/navo/IAS_nlomw12912mooper.gif)

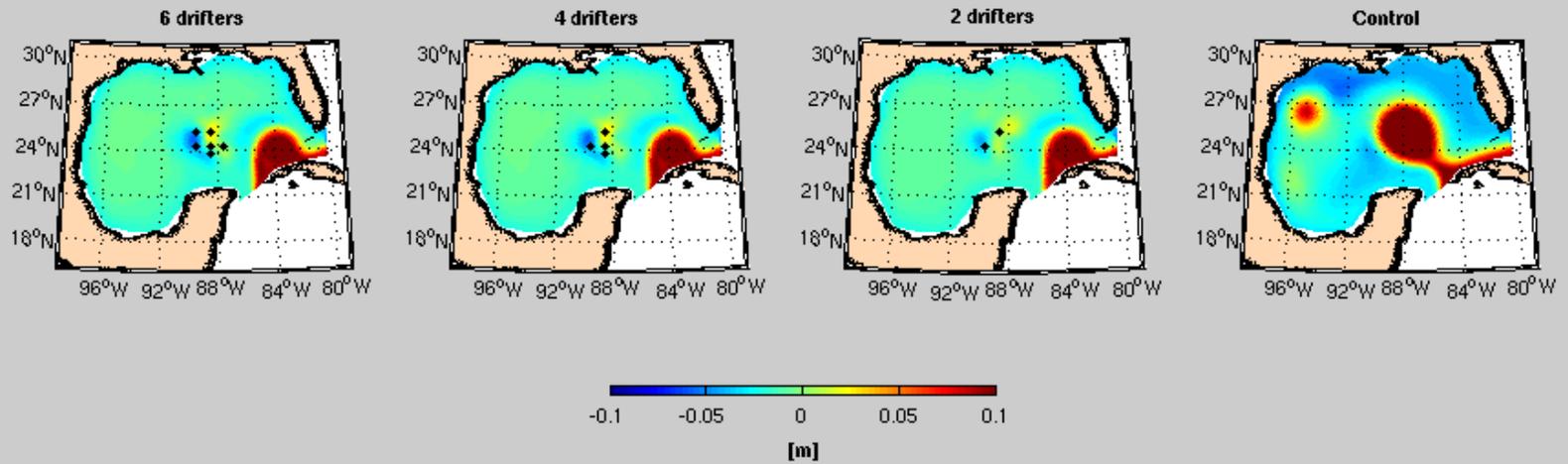
$$\mathbf{u}(\mathbf{r}_{D,j}, t) = \frac{d}{dt} \mathbf{r}_{D,j}$$



$$\int_{t_{k-1}}^{t_k} \mathbf{u}(\mathbf{r}_{D,j}, \tau) d\tau = \mathbf{r}_{D,j}(t_k) - \mathbf{r}_{D,j}(t_{k-1})$$

Data: <http://www.aoml.noaa.gov/phod/dac/dacdata.html>  
Special Thanks to Ed Ryan

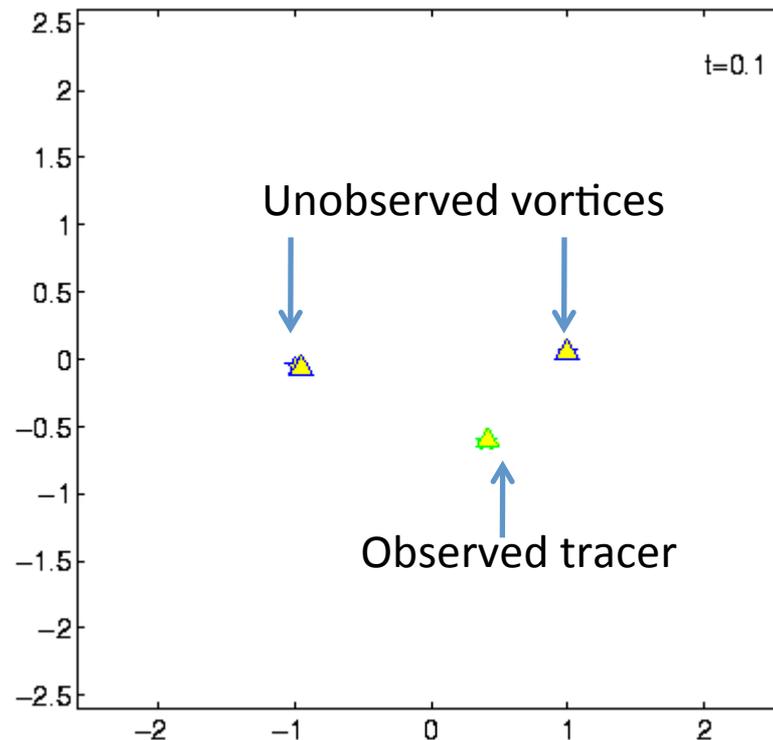
# Proof of Concept



# Challenge: Handling of Nonlinearity in Observation Operator

- ◆ Data assimilation grew up with quasi-linearity in mind
  - Nonlinearity in dynamics: Ensemble Kalman filter, Particle filter
  - Nonlinearity in observation operator: Handling of Chaos
    - Quality control requires extra steps

## ◆ Simple demonstration



# Quality Control of Data Assimilation Products

- ◆ Background: Global Ocean Data Assimilation Experiments (GODAE)
  - Initiated to lead the way in establishing global operational oceanography in 1997 as the acknowledgment of the need for better ocean observations and ocean forecasts and with the scientific and technical opportunity that readily available satellite data had delivered.
  
- ◆ Main Objectives
  1. To demonstrate operation ocean system in action
  2. To assess the quality of hindcast ocean products
  3. To perform the intercomparison among the different operational centers
  4. To promote validation and intercomparison as part of future ensemble multi model forecast applications.

# Quality Control of Data Assimilation Products

- ◆ Quality control in GODAE framework
  - Various ocean data quality-control procedures are used by GODAE systems to ensure that erroneous data are not assimilated. Some systems use externally processed observations, while other systems have developed their own automatic quality-control procedures.
  - For systems executed in reanalysis mode, the observational data have often undergone more extensive delayed-mode, scientific quality-control procedures that are not available in near-real time.
- ◆ New perspective: quality control of data assimilation product
  - Intercomparison-metric

# Summary

- ◆ Ocean data assimilation is relatively new, and may have different
  - Principal goals
  - Scales
  - Observations
- ◆ Conceptually, ocean data QC and atmospheric data QC are similar, we have to handle for
  - Individual
  - Data sets
  - Data types
- ◆ Observations are extremely important in ocean data assimilation
  - Number is limited
  - Inhomogeneous in time and space
- ◆ New types of observations are available
  - New types of QC: for example, QC for chaotic data (e.g., Lagrangian data)
  - Observing system design can be as important as the observed data themselves
- ◆ New prospect: Quality control of data assimilation products (overall)