Assimilation of VIIRS and AVHRR SST with Chesapeake Bay Operational Forecasting System

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Outline

- Project brief introduction and objectives
- Comparison of VIIRS/AVHRR SST with in-situ observations
- 4DVAR data assimilation with CBOFS
- Results-Comparison with Observations
- Summary and conclusion

Scientific Basis/Approach

- Temperature and salinity are critical in understanding the coastal ocean and ecosystems, yet difficult to forecast synoptically
- NOAA's operational Chesapeake Bay Operational Forecasting System (CBOFS) forecasts T/S, but there exist bias and deviations from measurements, would benefit from the assimilation of satellite-derived SST.
- Several data assimilation techniques available; evaluate whether 4D-VAR (Moore et al.,2011) or LETKF (Hunt et al. 2007) is better for assimilating SST retrievals into CBOFS
- Satellite SST retrievals have previously been assimilated into hydrodynamic models, but not operationally by NOAA

Overall Goal:

- Determine whether 4DVAR or LETKF should be used when assimilating VIIRS SST, together with other available observations, into CBOFS.
- Quantify the improvement of retrievals from VIIRS vs AVHRR SST.

Only 4DVAR results are reported here.

Funded by Joint Polar Satellite System Proving Ground and Risk Reduction Program.

Objective

- Assimilating VIIRS SST into CBOFS to improve model performance using 4DVAR. Compare/Validate with independent/in-situ observations.
- Comparing different data assimilation methods.

  4DVAR versus LETKF
- Assimilation of VIIRS SST and AVHRR SST L2 products with CBOFS

Chesapeake Bay Operational Forecasting System (CBOFS)

- Operationally Running at NOAA NOS CO-OPS

  Regional Ocean Modeling System (ROMS) 3.0 with resolution 33 m to 4 km.

  Every 6 hours, forecast up to 48 hours for water temperature, salinity, currents, sea level.

  Initial error for temperature is less than 1^{o} C and salinity less than 3.

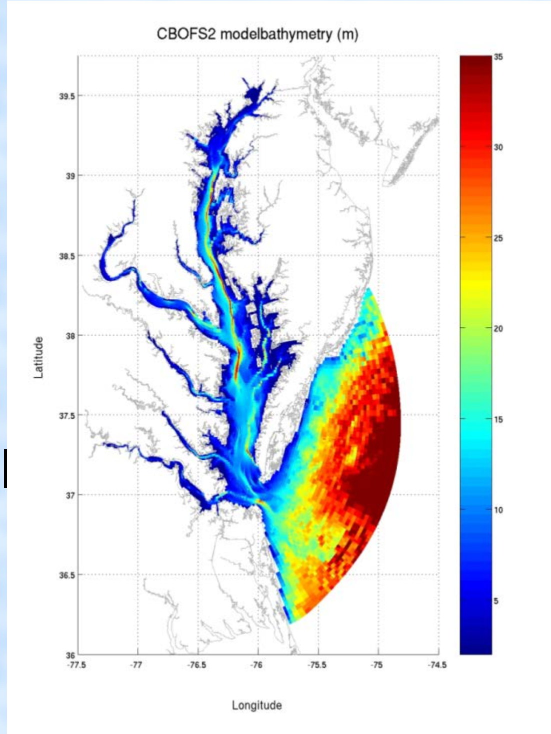
- Surface and open boundary forcing

  North American Mesoscale Forecast System (NAM).

  USGS river flow, Global Real Time Ocean Forecast System (RTOFS), ADCIRC tides, sea levels at two observational stations (Duck and Ocean city).

  Along with time, errors on forcing can make the model bias increase compared to observations.

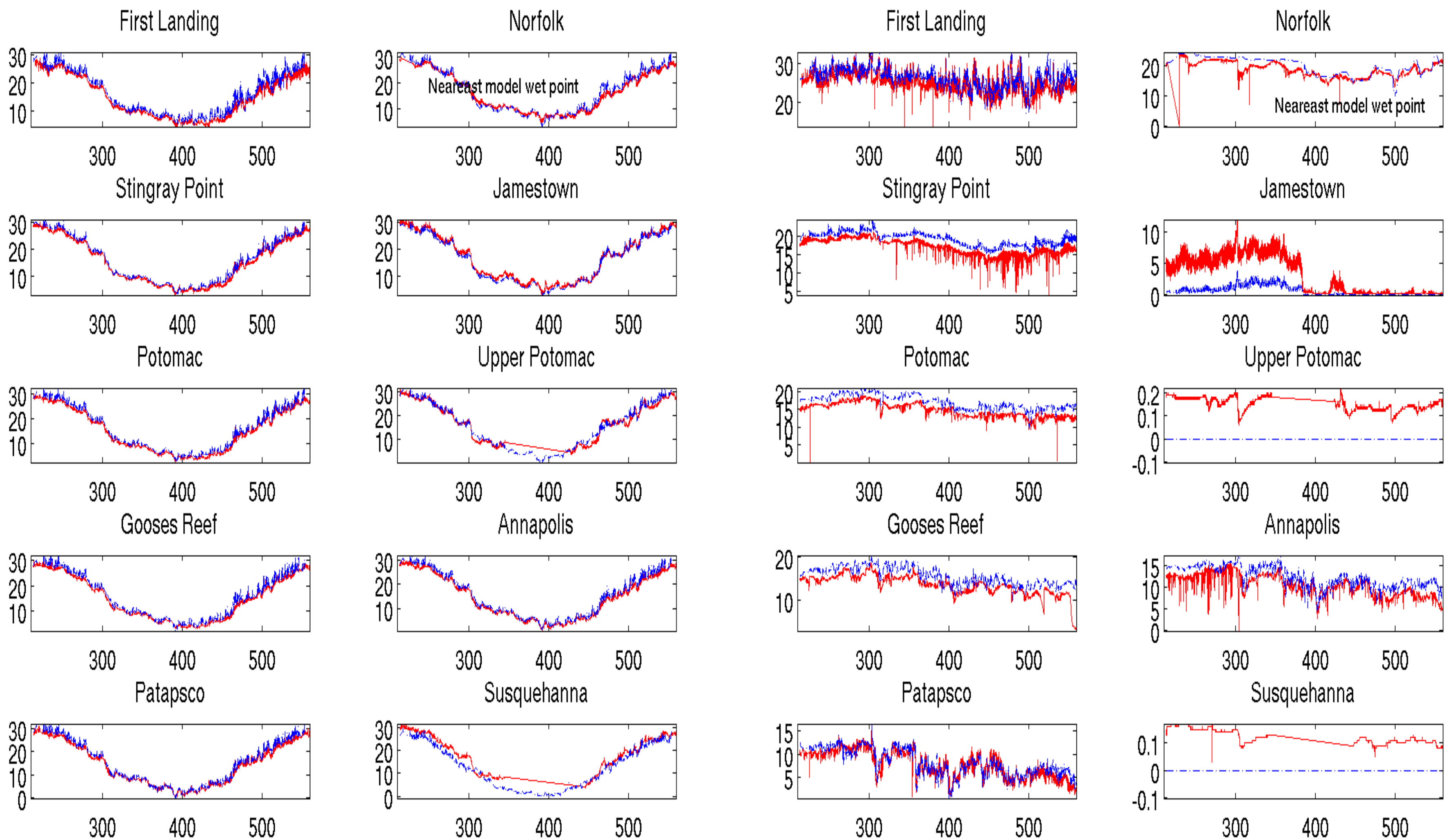
- No data assimilation setup.



CBOFS Comparison with Observations (CBIBS)

Surface Temperature

Surface Salinity



Days starting from 01/01/2012 (Red Line: CBIBS; Blue Line: CBOFS,08/2012-07/2013)

VIIRS SST

- **Suomi NPP VIIRS SST(L2 SWATH data) for Data Assimilation**

  Overpass Chesapeake Bay twice per day with high resolution of 750m.

  Operational NOAA/NESDIS/STAR ACSPO products.

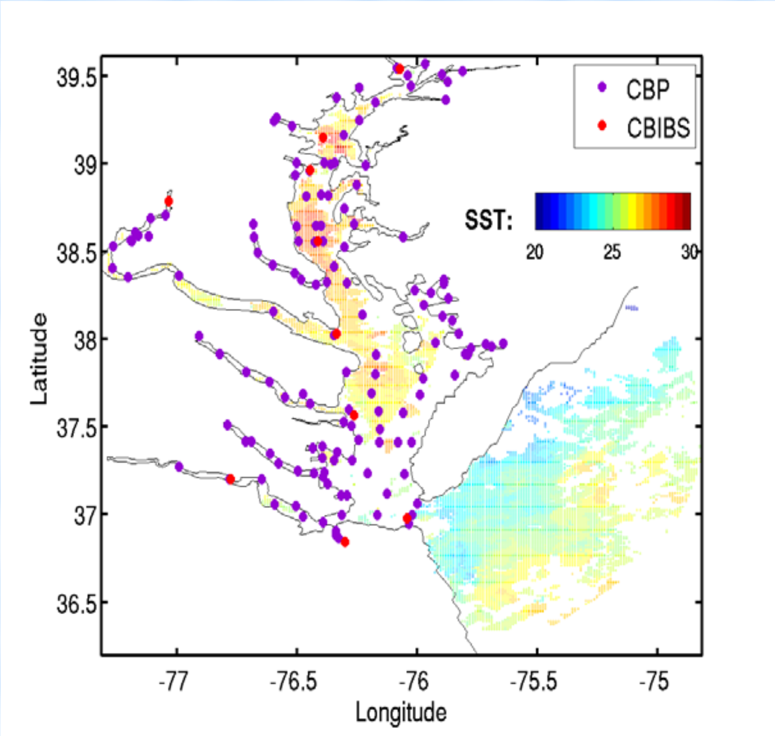
  Available datasets (05/2014- present)

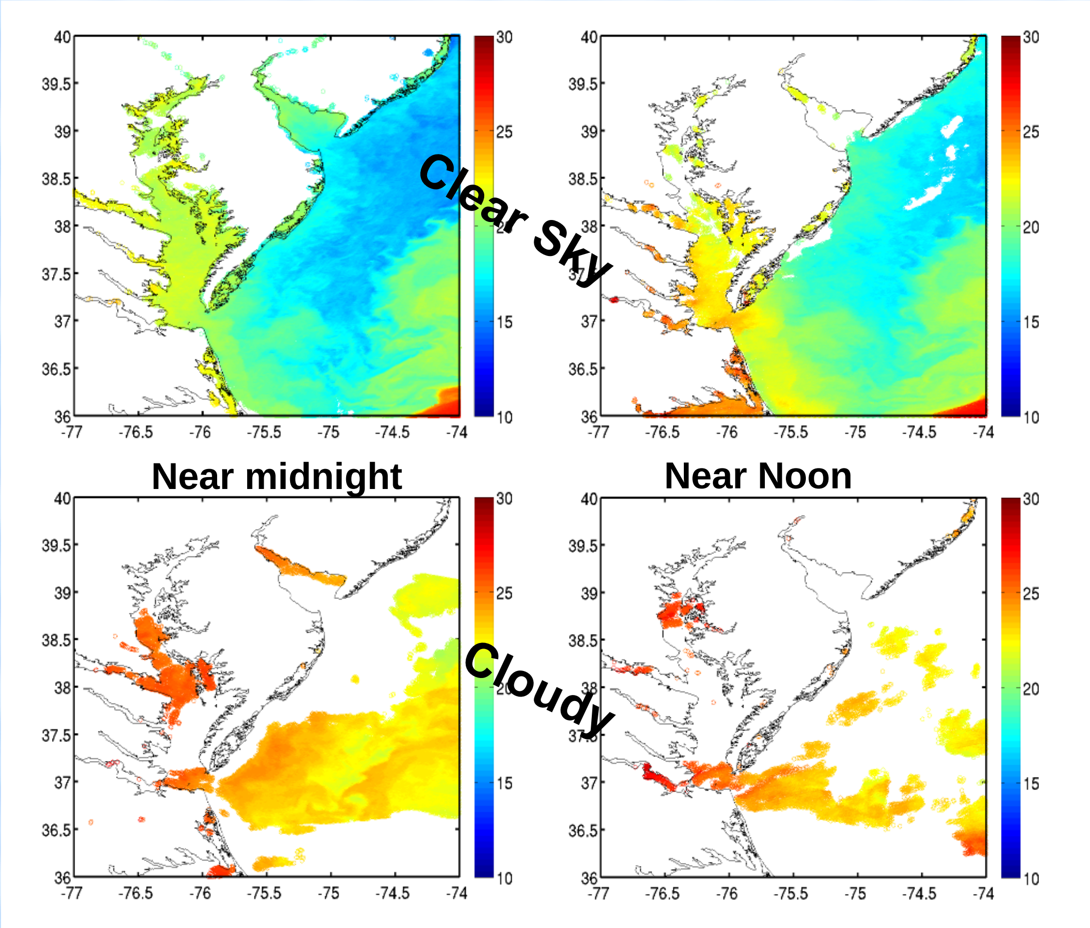
- **Chesapeake Bay Interpretive Buoy System (CBIBS)**

  15 minutes surface T/S from 11 stations

- **Chesapeake Bay Program(CBP) T/S**

  Two-four weeks CTD casting of T/S





AVHRR SST

- **AVHRR SST**

  Includes NOAA-15, NOAA-18, NOAA-19 satellites, MetopA and MetopB over Chesapeake Bay area.

  Near nadir resolution about 1.1km.

  Each satellite overpasses the Chesapeake Bay twice per day, which has high temporal resolution.

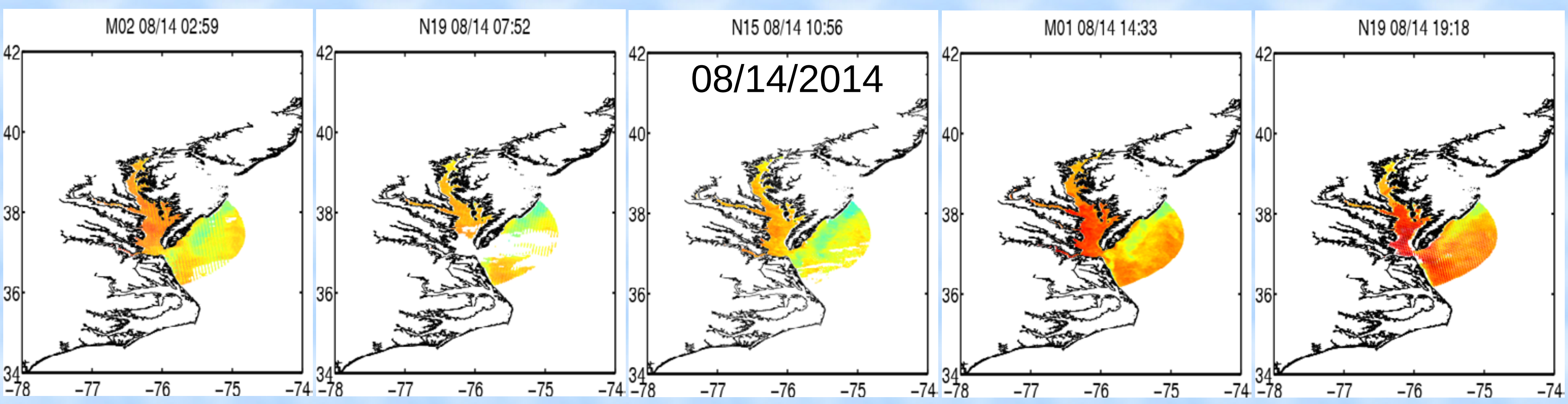
  This data sets are available from NOAA coastal watch website and NOAA CLASS.

- **Daily composite vs single-time SST**

  Daily composite are simple mosaic of multiple SST observations from different satellites in each day with higher resolution. Useful for seasonal overlook or long term variations. Not suitable for coastal/estuaries data assimilation (e.g Data Assimilation) due to supression of diurnal variation.

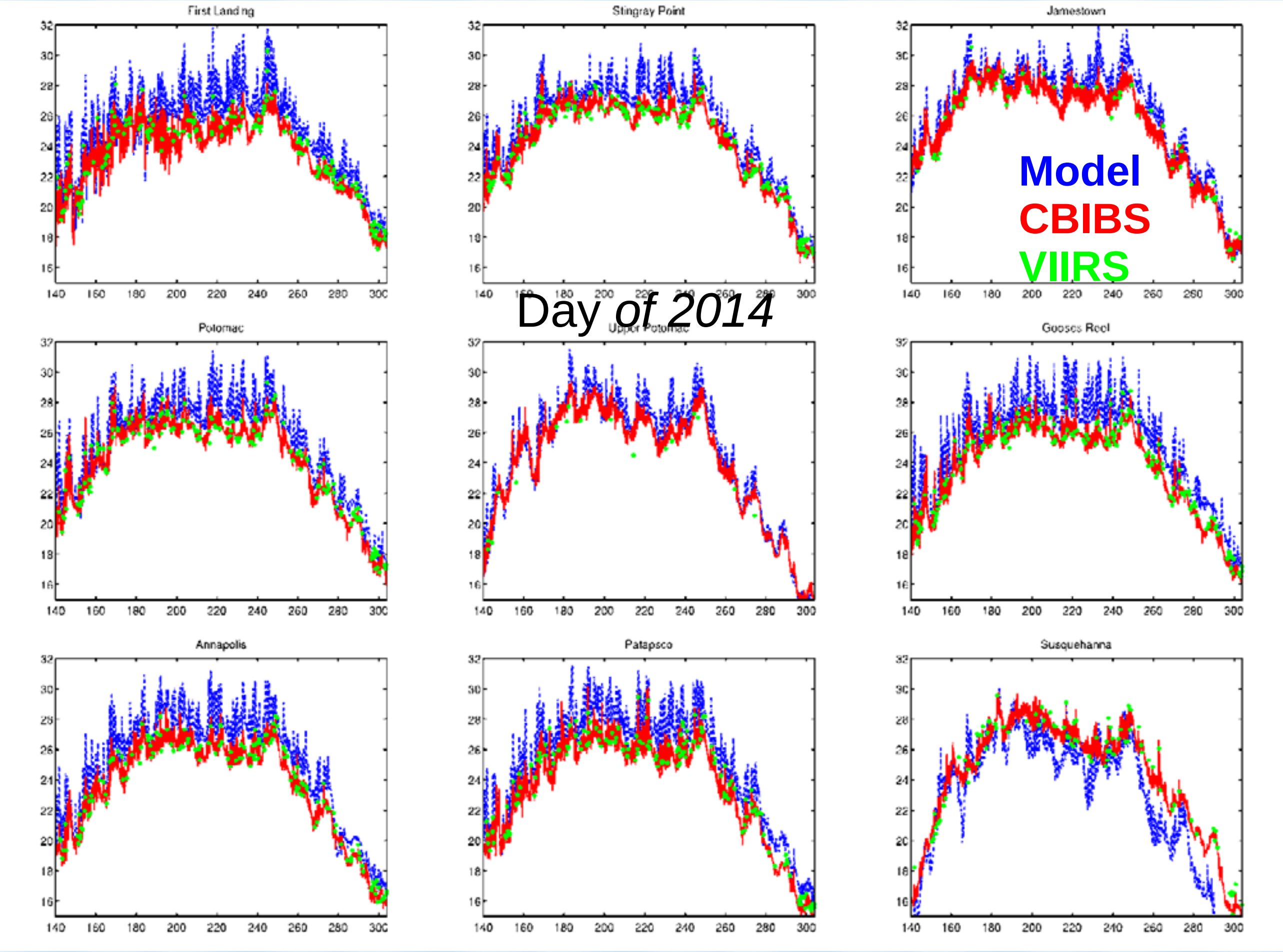
  SST images from each satellite provides exact timing and pixel locations. These instant SST observations from different satellites (including VIIRS SST) can be used for direct data assimilation to improve model SST.

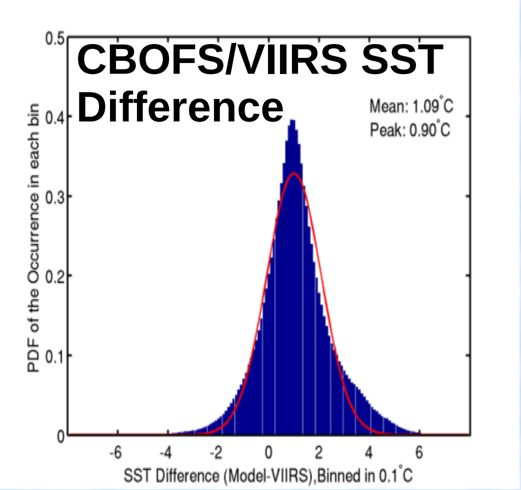
Multiple Observations in one day from different satellites at different hours (in CBOFS model domain)

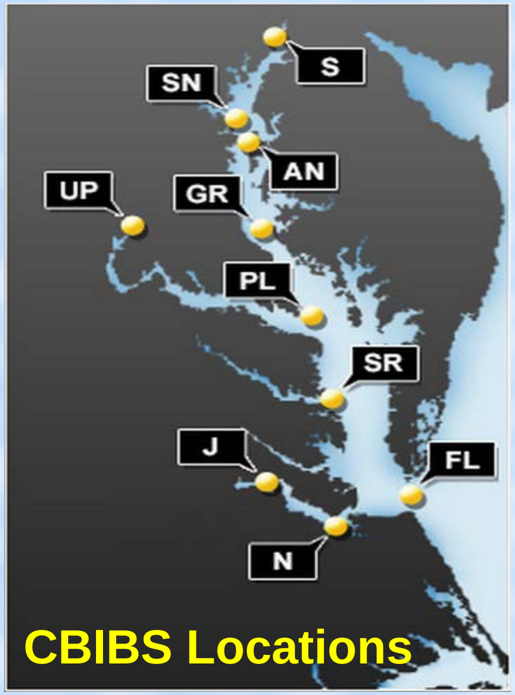


MODEL/VIIRS/CBIBS SST Comparison

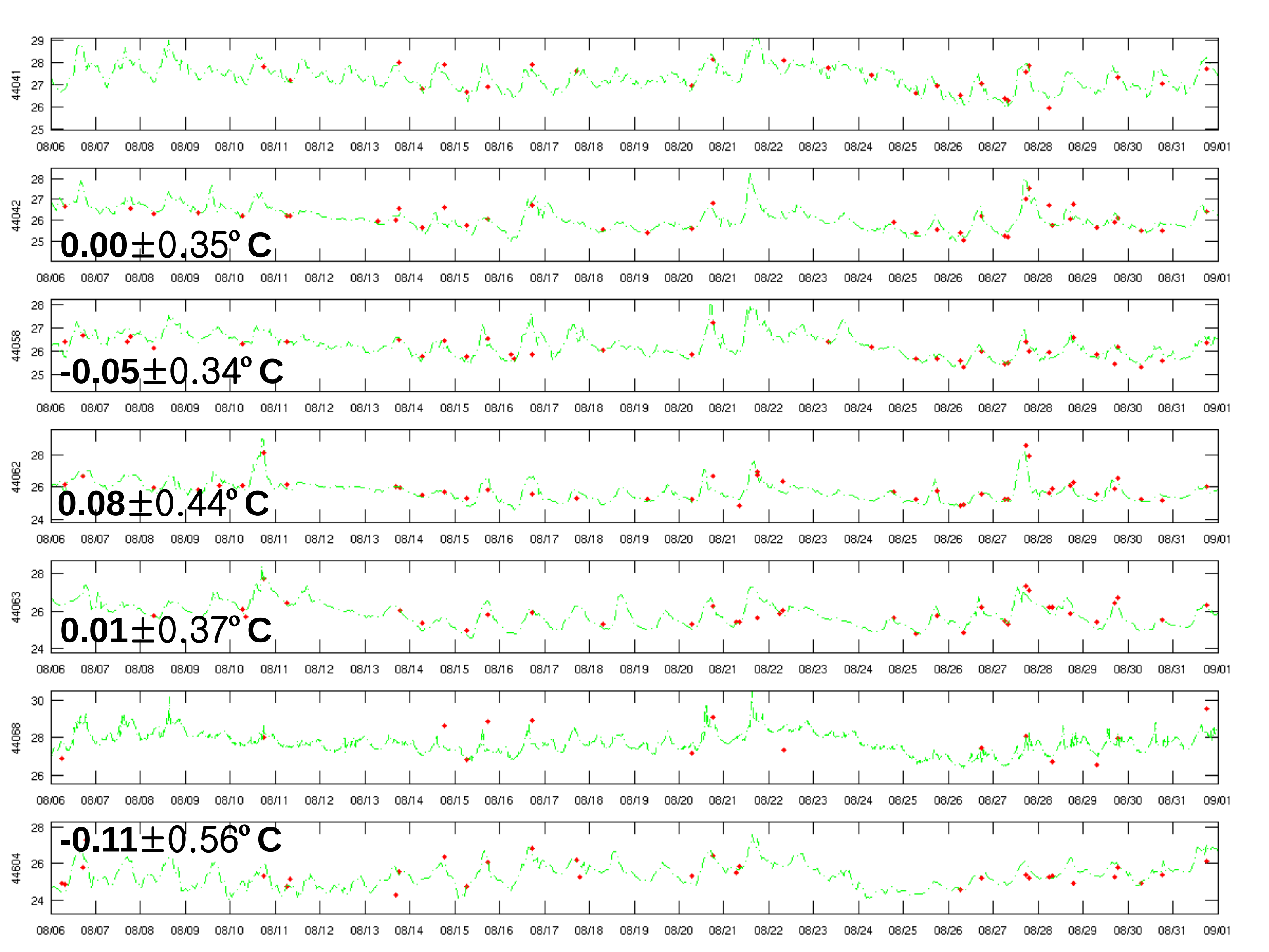
- **VIIRS SST is close to Buoy SST (0.16±0.60° C).**
- **CBOFS SST bias: 0.7° C~1.4° C for CBIB stations.**
- **CBOFS SST bias: 1.09° C for VIIRS SST.**



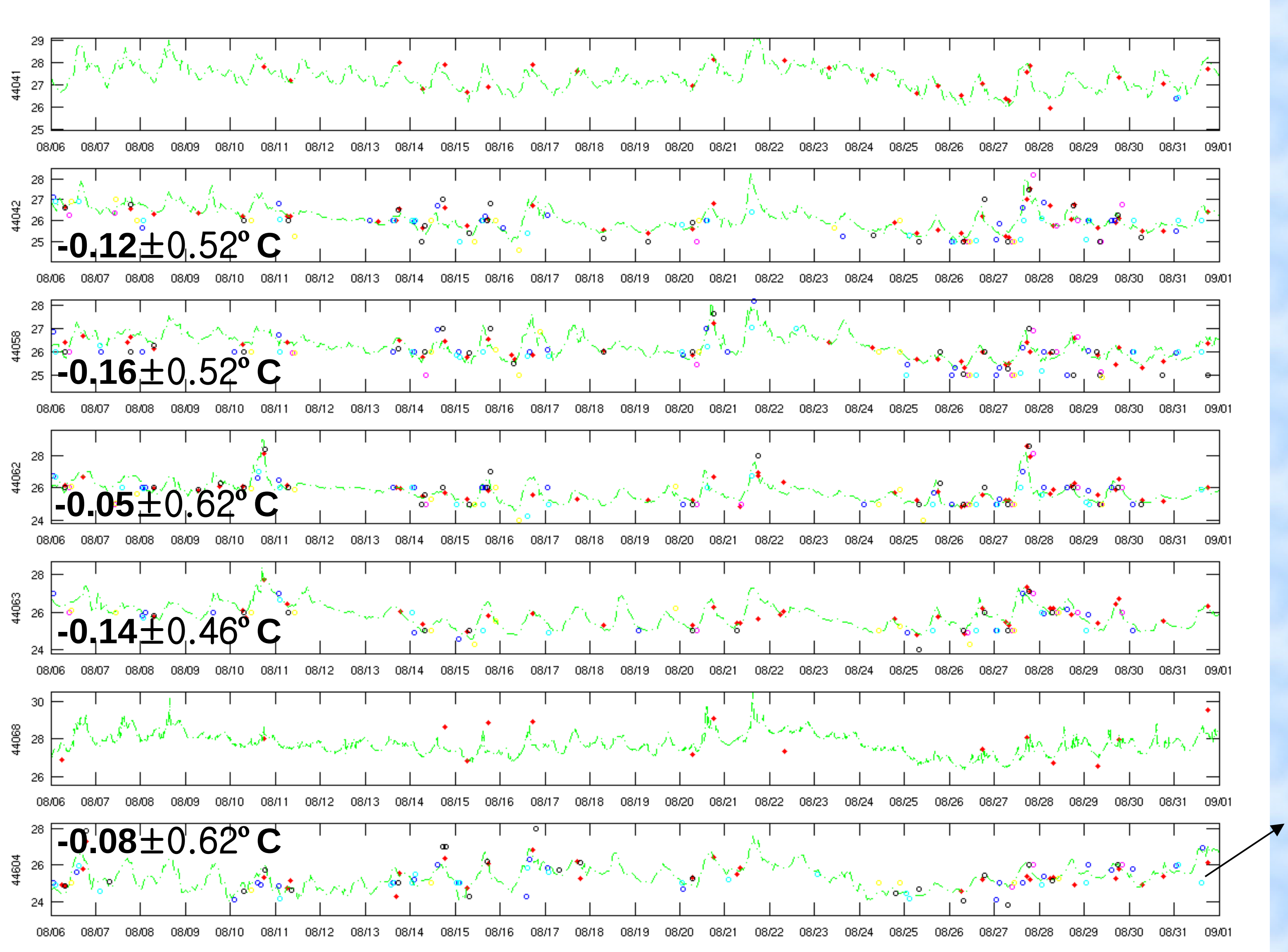




VIIRS SST 08/2014



VIIRS SST & AVHRR SST



AVHRR SST has higher (also negative) bias with higher stand deviations than VIIRS SST, not all CBIBS stations have enough AVHRR SST data due to their locations.

ROMS 4DVAR

- **Incremental Strong Constraint (I4DVAR)**

  Primal form, Initial conditions, surface forcing, open boundary conditions

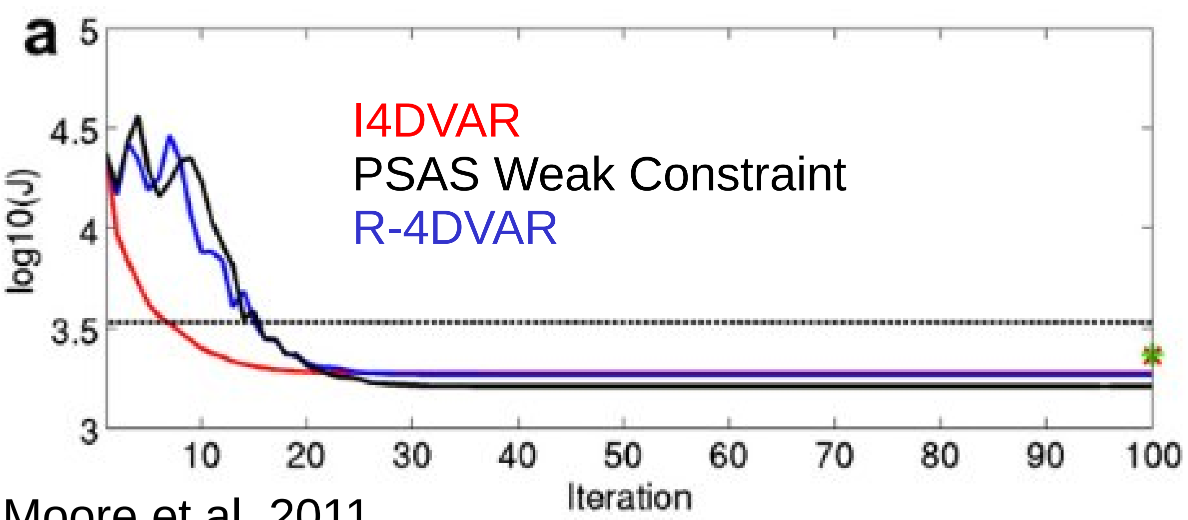
  Lanczos conjugate gradient solver.

- **Physical-Space Statistical Analysis (PSAS)**

  Dual forms, in model and observational spaces.

  Strong constraint; Weak constraint (Considering model errors).

- **Representer 4DVAR (R4DVAR)**



Moore et al. 2011

I4DVAR and adjust initial condition only for this study.

I4DVAR Preparation

- $J(\delta x) = \frac{1}{2}\delta x^T B^{-1}\delta x + \frac{1}{2}\sum (H\delta x - y)^T O^{-1}(H\delta x - y)$

Background Error Covariance

Observational Error Covariance

$$B = K_b \Sigma C \Sigma^T K_b^T$$

Balanced Operator

Standard deviation

Correlation Matrix

✓ Estimated from SST and CTD Obs

Horizontal and Vertical Decorrelation Length Scale

Calculated from Forward ROMS

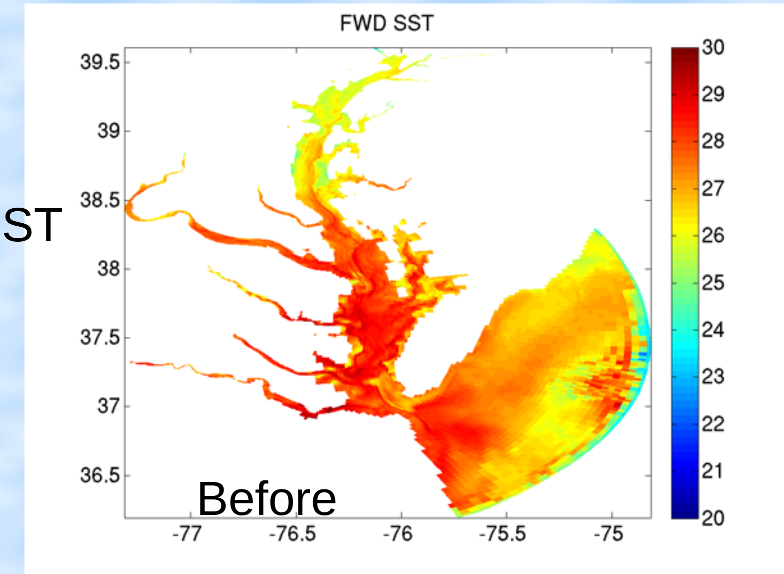
ROMS NORMALIZATION OPTION

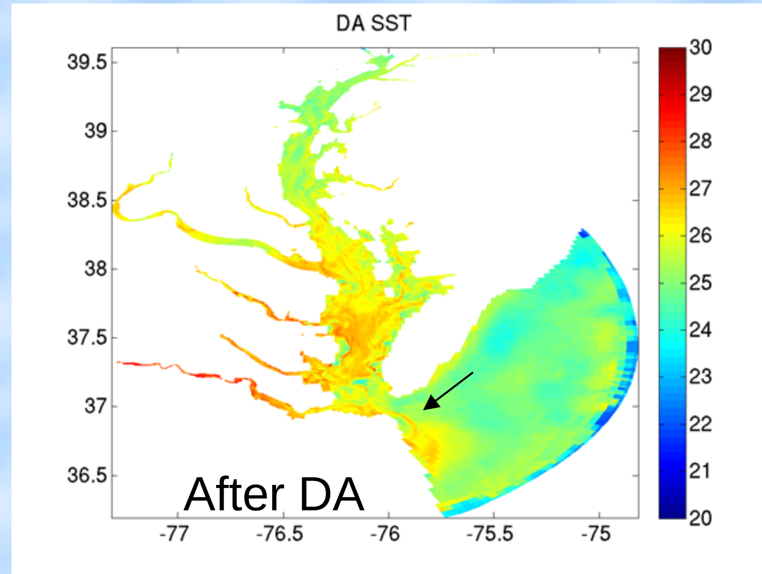
✓ One year simulation, detide, remove seasonal cycles

✓ Normalized coefficients calculation
Only needs model grids and length scales

Adjustment of SST

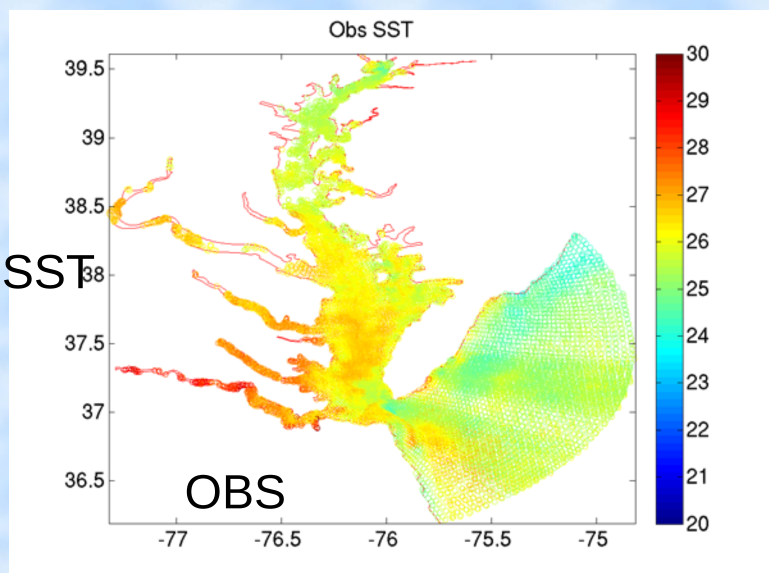
FWD
Initial SST

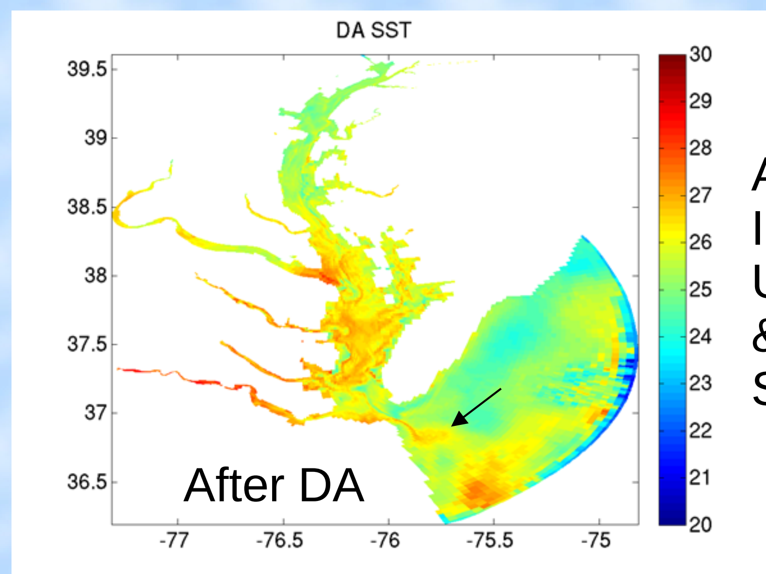




Adjusted
Initial SST
Using VIIRS
SST only

VIIRS &
AVHRR SST





Adjusted
Initial SST
Using VIIRS
& AVHRR
SST

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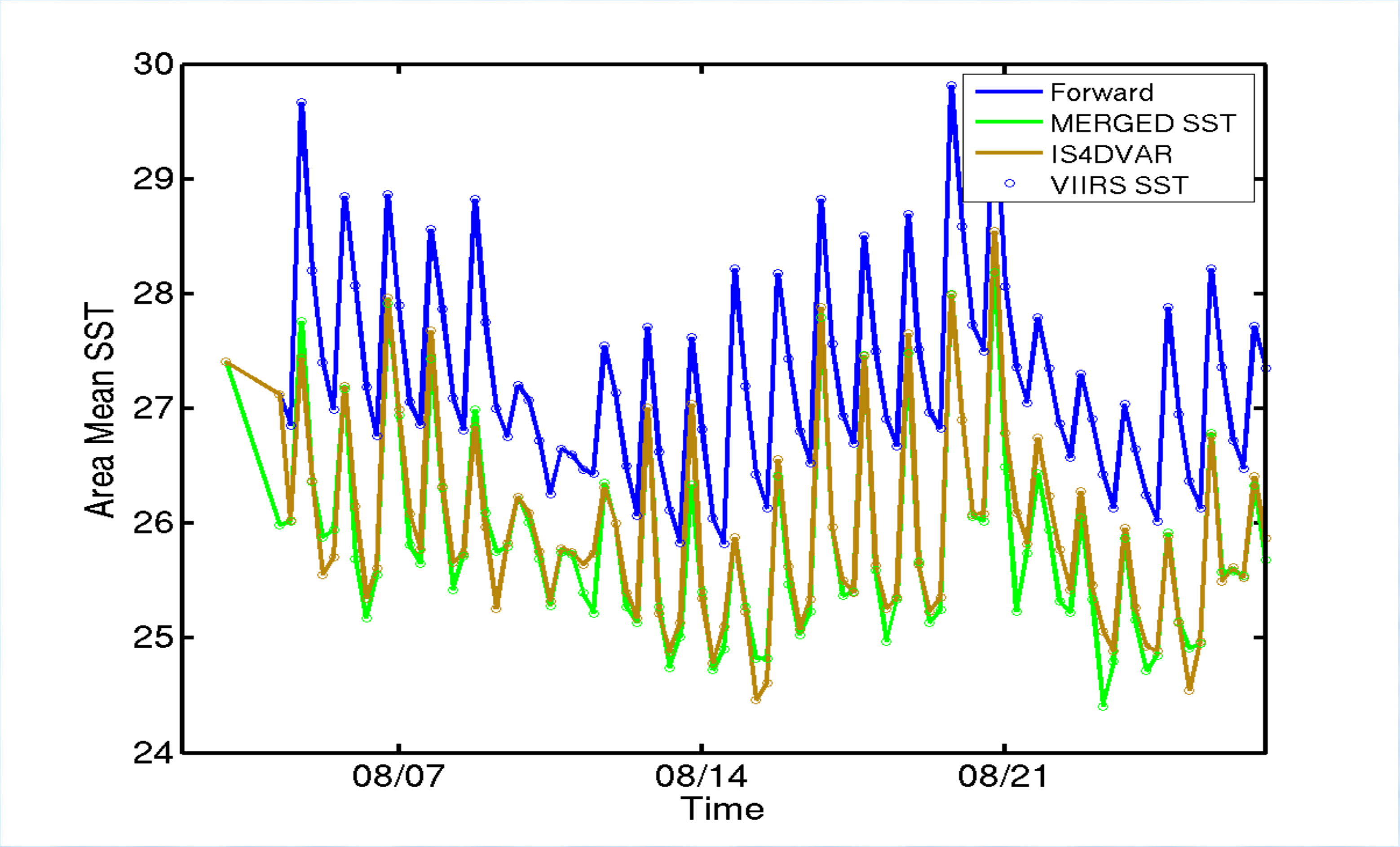
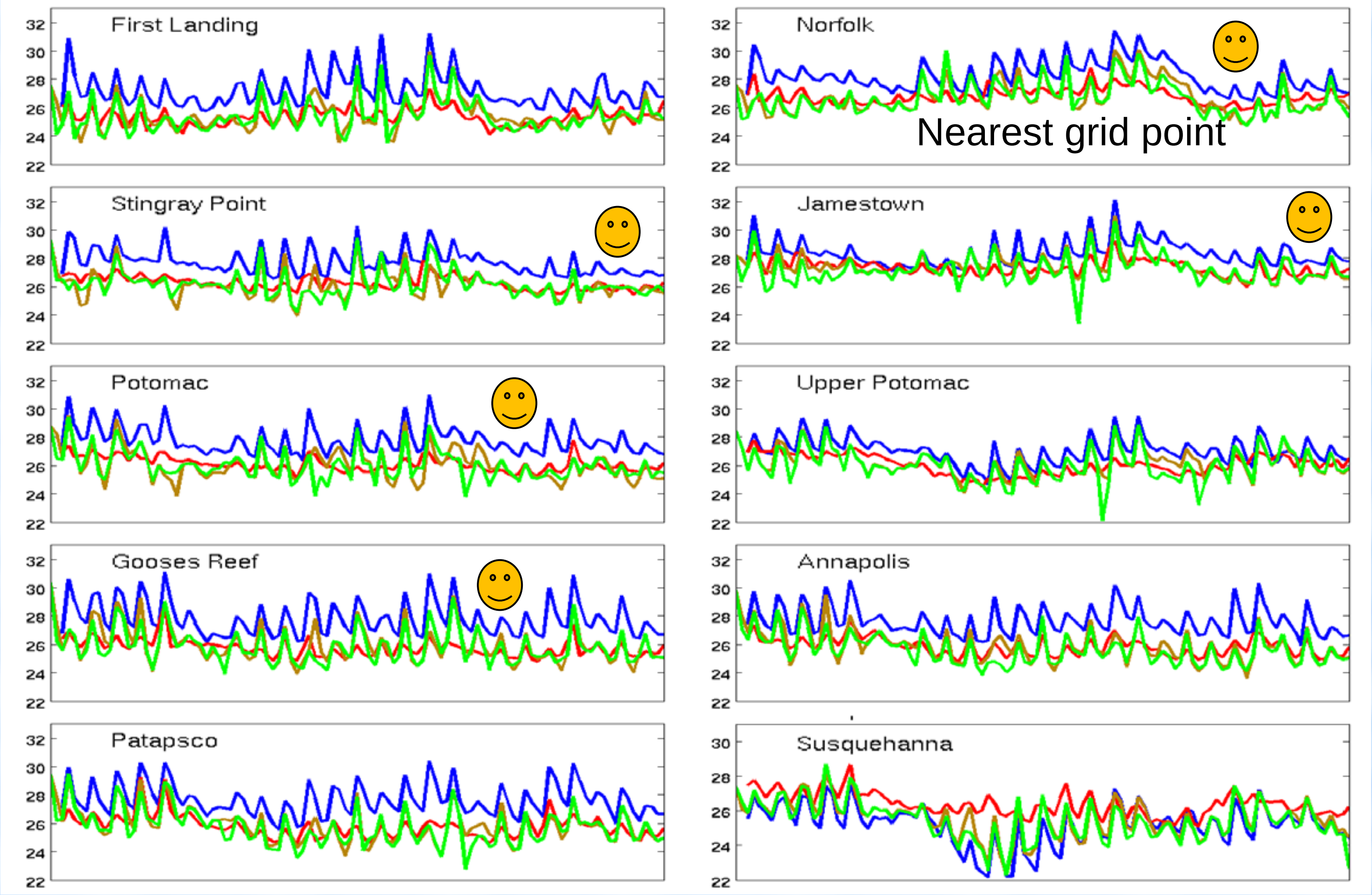
One Month Sequential Run with AVHRR & VIIRS SST of I4DVAR



Mean FWD SST: 27.4º **C;** Mean DA SST using AVHRR & VIIRS SST: 26.1º **C**; Mean DA SST using VIIRS SST only 26.3º **C**; VIIRS SST Mean: 25.8º **C**

I4DVAR (Comparison at CBIBS Stations)

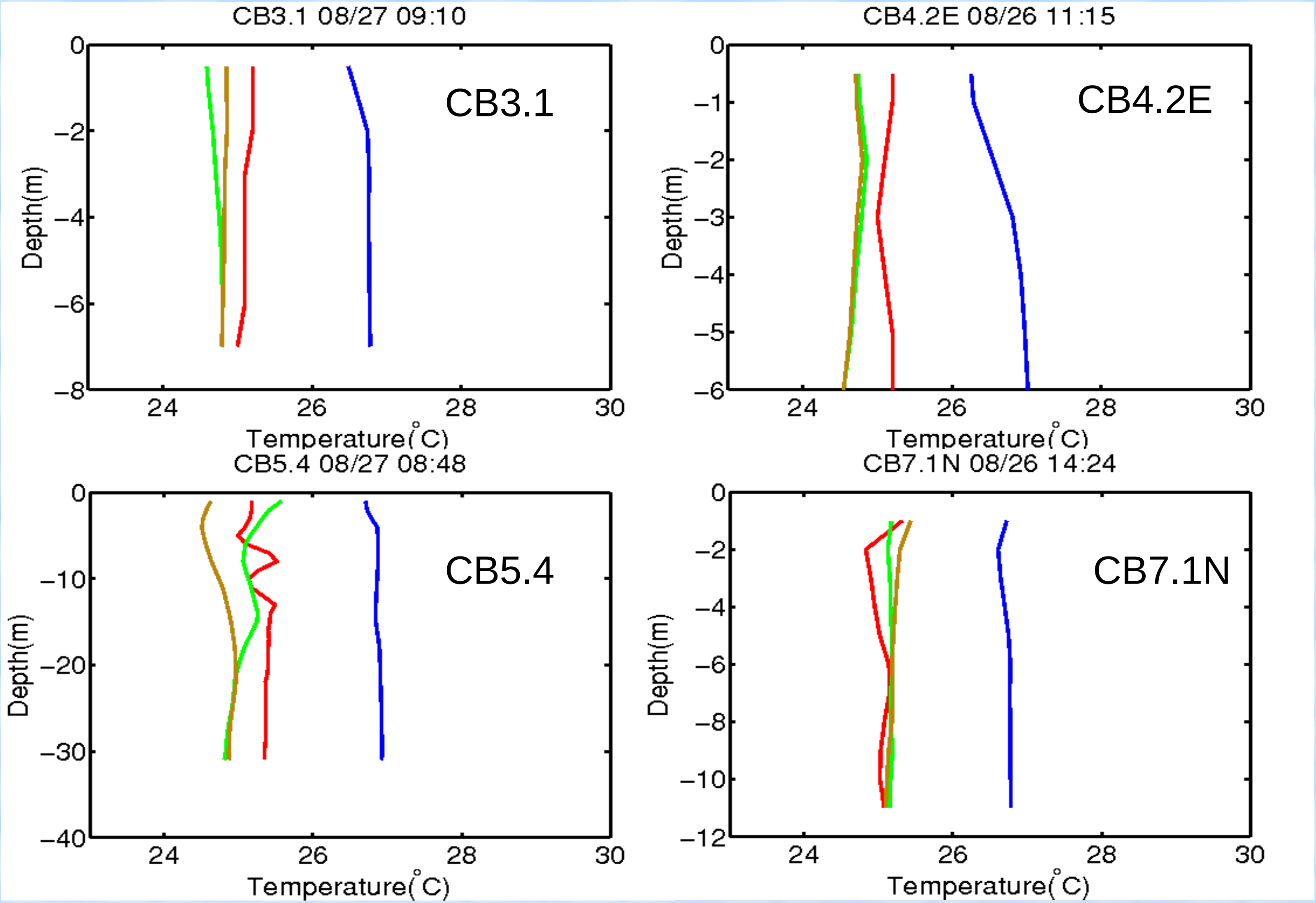
CBIBS; Forward Model; DA with Both SST; DA with VIIRS SST



Have AVHRR observations nearby

After assimilating VIIRS SST, Bias are within 0.2° C for all stations except Susquehanna station. Using VIIRS and AVHRR SST , bias are within 0.23° C, but more stations have negative bias. Both difference with a mean standard deviation of 0.88° C

Comparison with CBP Observations



Red: Observation; Blue: Forward Model; Green: AVHRR &VIIRS DA; Gold: VIIRS DA

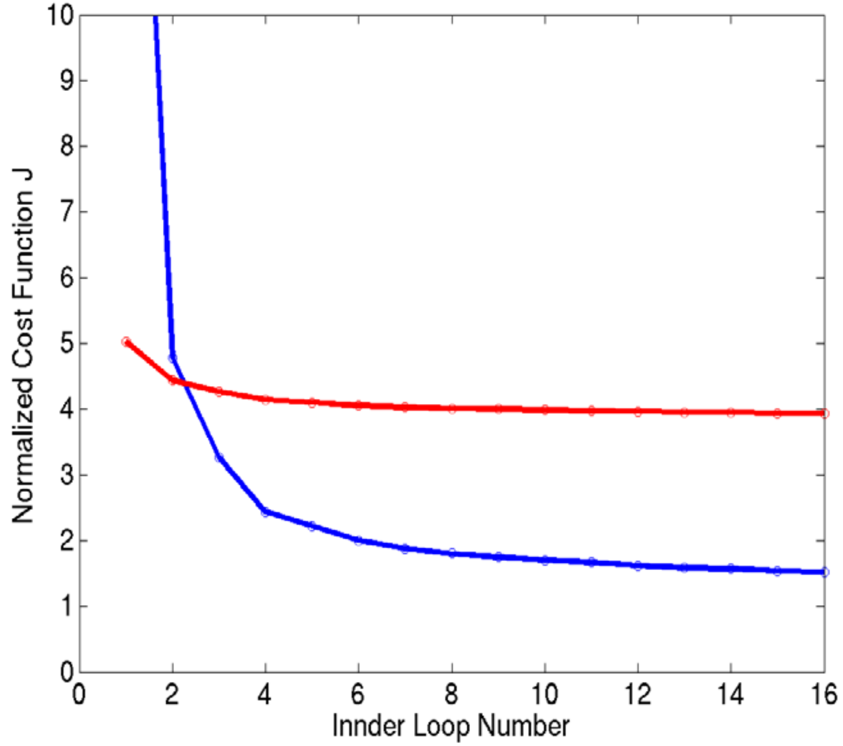
Temperature profile changes with assimilation of different datasets. More constraint on the vertical profile might be needed.

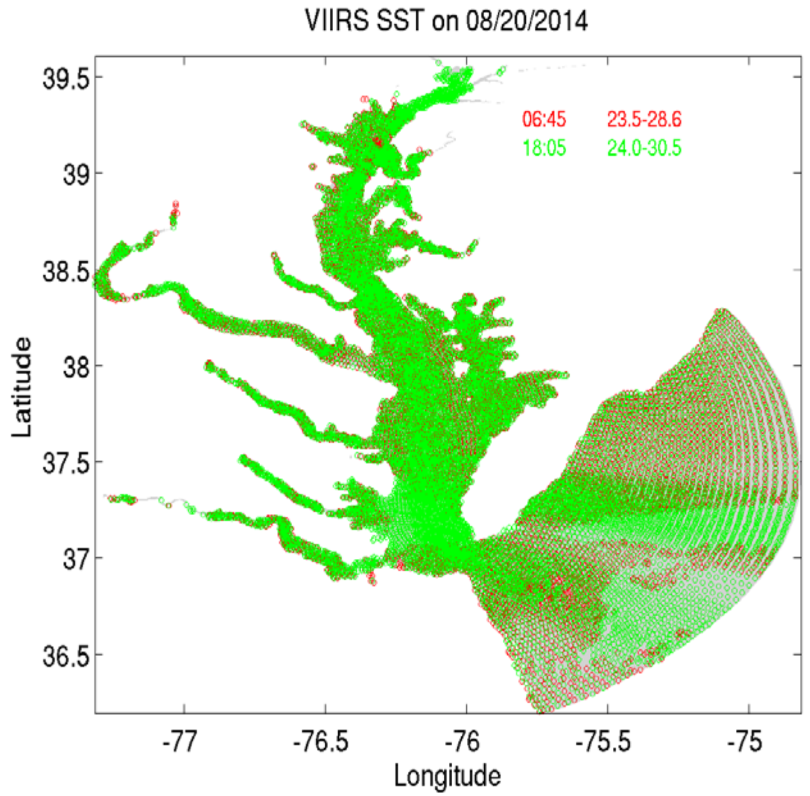
Summary

- Comparison of VIIRS SST and different AVHRR SST L2 products with buoy observations shows that VIIRS SST is generally better than AVHRR SST both in bias and standard deviation over the Chesapeake Bay area.
- L2 SST preserves the original observation without interpolation and smoothing, more suitable for estuaries data assimilation than the gridded products. But this may need more quality control work.
- Assimilating AVHRR SST and VIIRS SST from different satellites can increase the model ability in resolving fine scale structure within diurnal variation.
- Assimilation of both AVHRR SST and VIIRS SST does not have significant improvement in terms of reducing bias than VIIRS SST only, likely due to larger errors and negative bias in the AVHRR SST in the Chesapeake Bay.
- DA with combined SST can partially improve stratification (more close to CBP profiles) in vertical than using VIIRS SST itself.
- Assimilation of SST products from different satellites using ocean model provides a way of blending of SST products, especially in estuaries.

Thanks!

Cost Function





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Two 6 hour assimilation windows

Cost Function (J) for total (blue) and tangent linear (red) model.

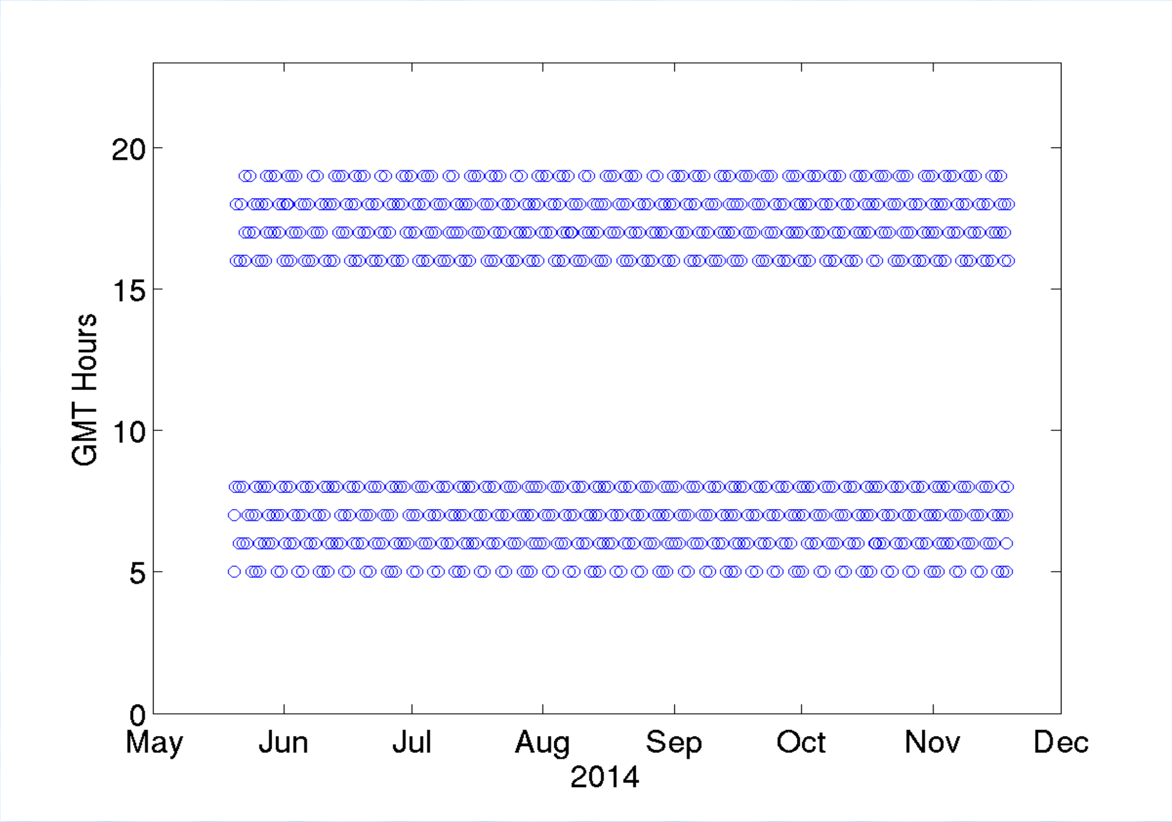
If very few numbers of observations, discarded.

VIIRS SST Time

- SNPP sun-synchronized satellite

Pass each location on a nearly fixed (local) time.

- Scanning Chesapeake Bay at:



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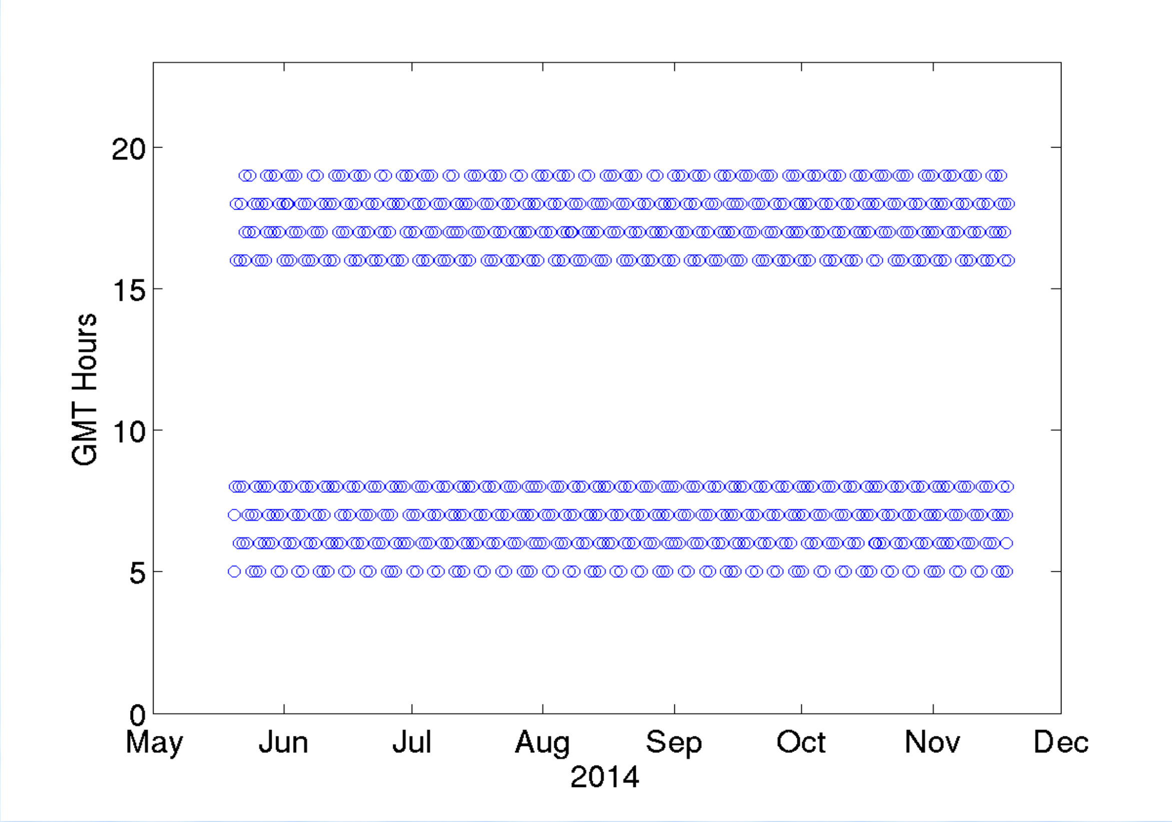
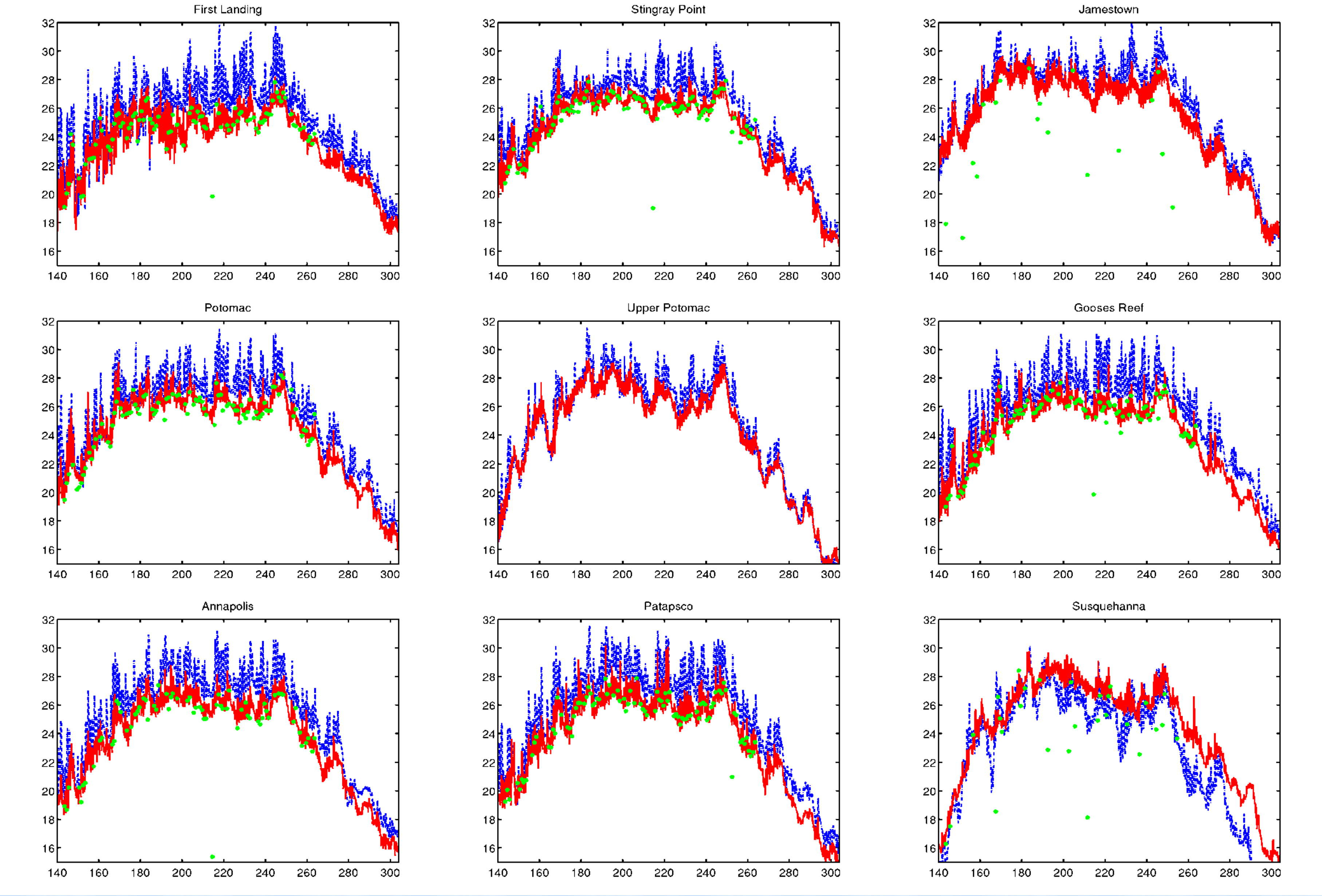


AVHRR SST at CBIBS locations



Blue: Model; Red: CBIBS; Green: AVHRR SST Day of 2014

Model/VIIRS/CBIBS SST

VIIRS SST-CBIBS SST

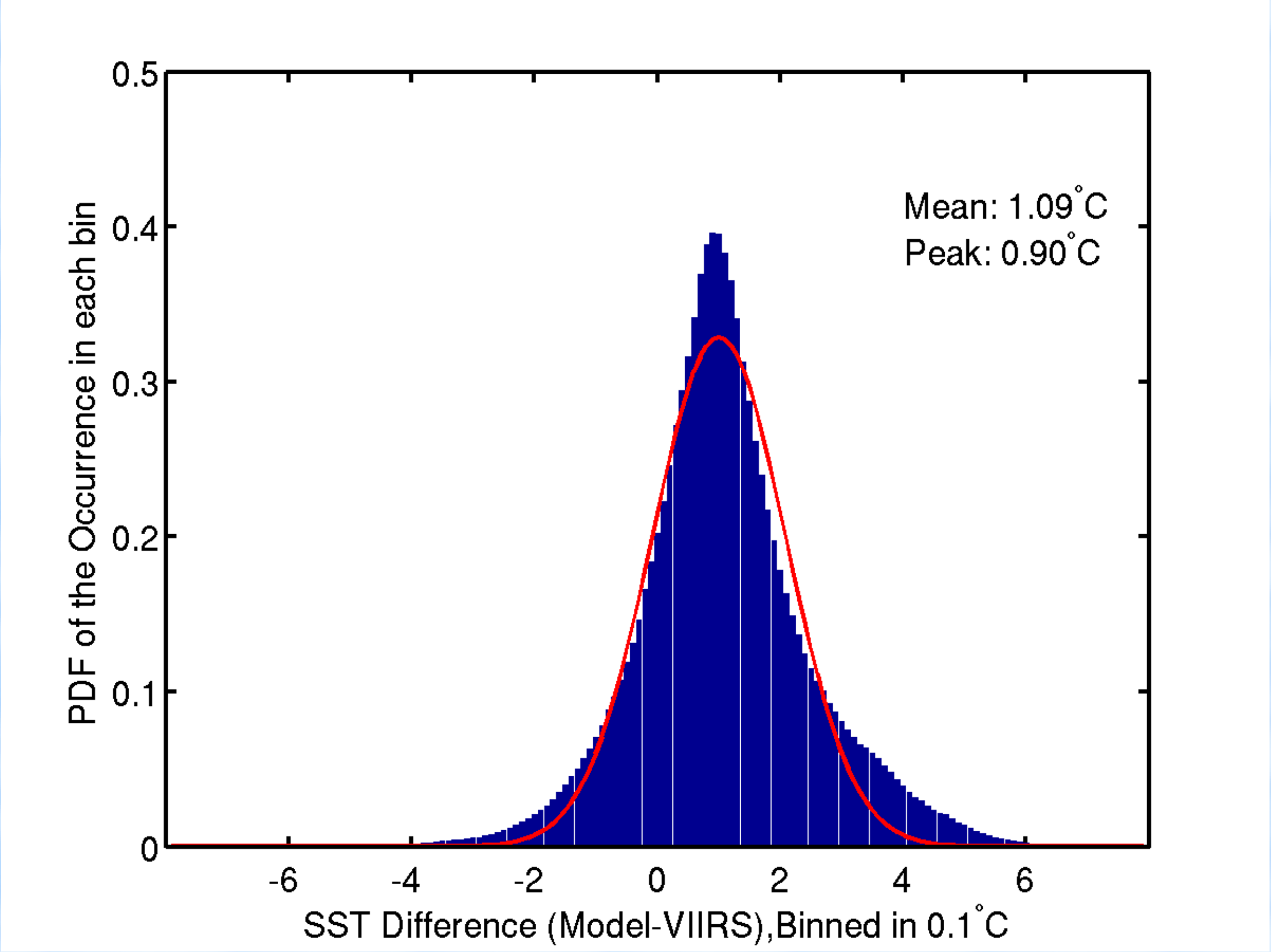
Stations	First Landing	Stringray Point	James town	Potomac	Upper Potomac	Gooses Reef	Annapolis	Patapsco	Susquehanna	RCU
SST Diff	0.14	0.15	0.09	0.17	-0.35	0.23	0.20	0.23	0.11	0.19
SST STD	0.72	0.47	0.39	0.57	0.57	0.53	0.41	0.52	0.58	0.60
TOTAL Number	173	176	54	163	19	187	153	165	88	26

VIIRS SST-Model SST

at CBIBS locations

Stations	First Landing	Stringray Point	James town	Potomac	Upper Potomac	Gooses Reef	Annapolis	Patapsco	Susquehanna	RCU
SST Diff	-1.40	-0.90	-0.56	-1.16	-0.47	-1.40	-1.37	-1.44	1.41	-0.29
SST STD	1.12	0.81	0.69	0.98	0.77	1.01	0.81	0.82	1.73	0.73
TOTAL Number	173	176	54	163	19	187	153	165	88	26

VIIRS SST Vs CBOFS SST

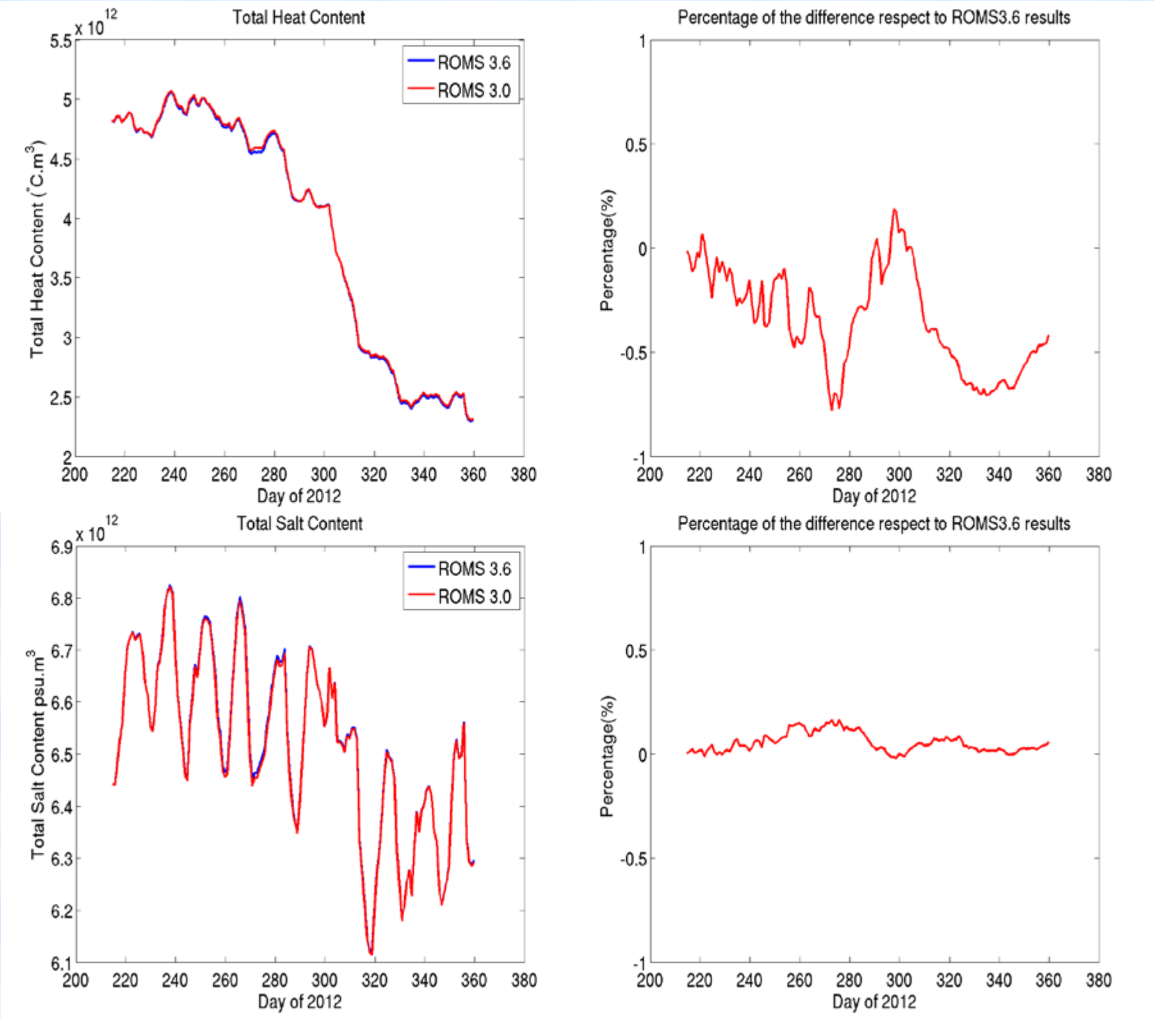


- Downloaded the VIIRS SST data

  From ftp://podaac-ftp.jpl.nasa.gov/allData/ghrsst/data/GDS2/L2P/VIIRS_NPP/OSPO/v2.3/2014/140/
- Rerun CBOFS from 05/21/2014 to current

Saved hourly temperature data and retrieved surface data.

Five Month Run (08/02-12/25/2012) validation of updating of ROMS



Open Boundary: in ROMS 3.0

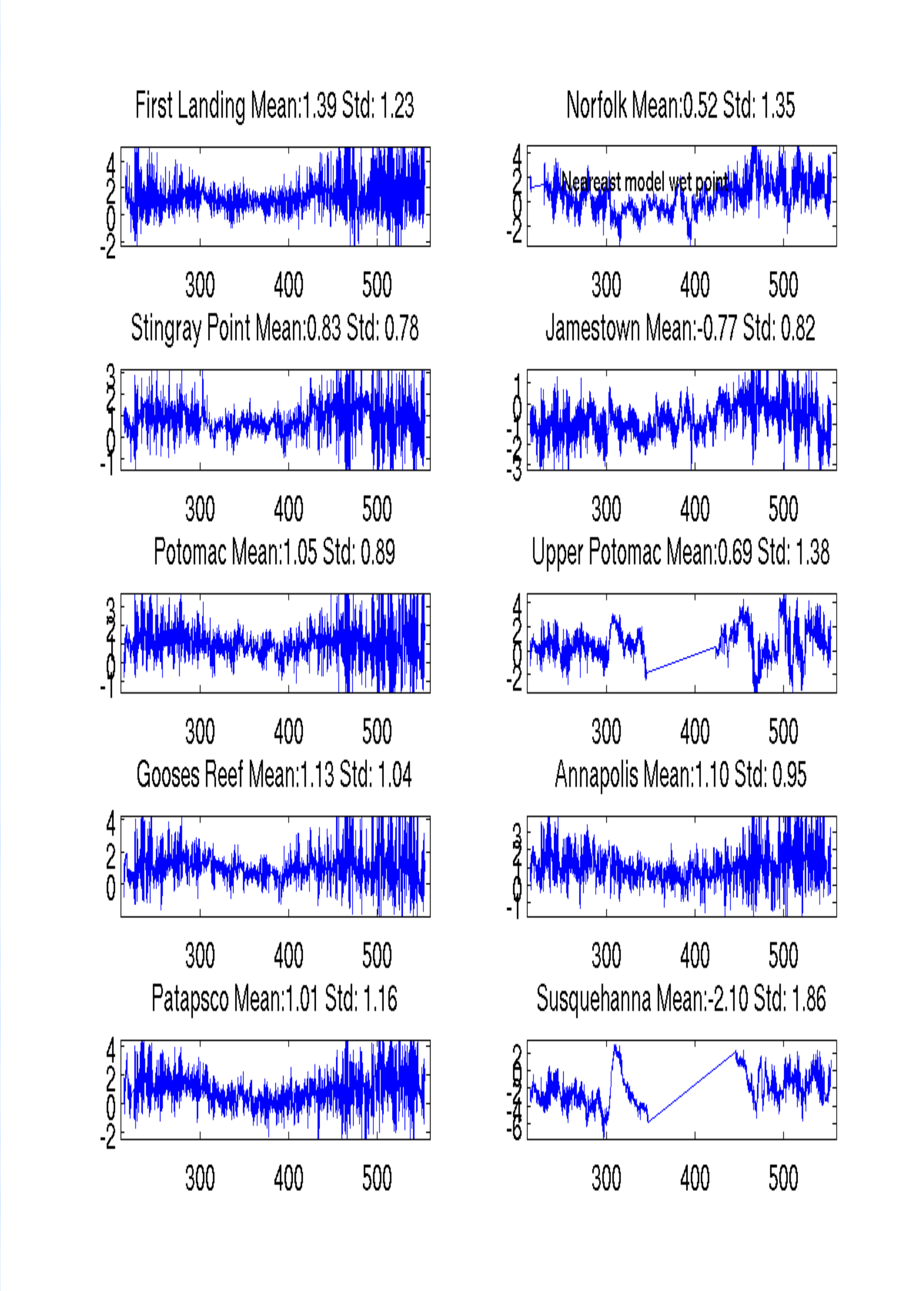
#define SOUTH_FSCLAMPED
#define SOUTH_M2REDUCED
#define SOUTH_M3RADIATION
#define SOUTH_TNUDGING
#define SOUTH_TRADIATION

Open Boundary: in ROMS 3.6

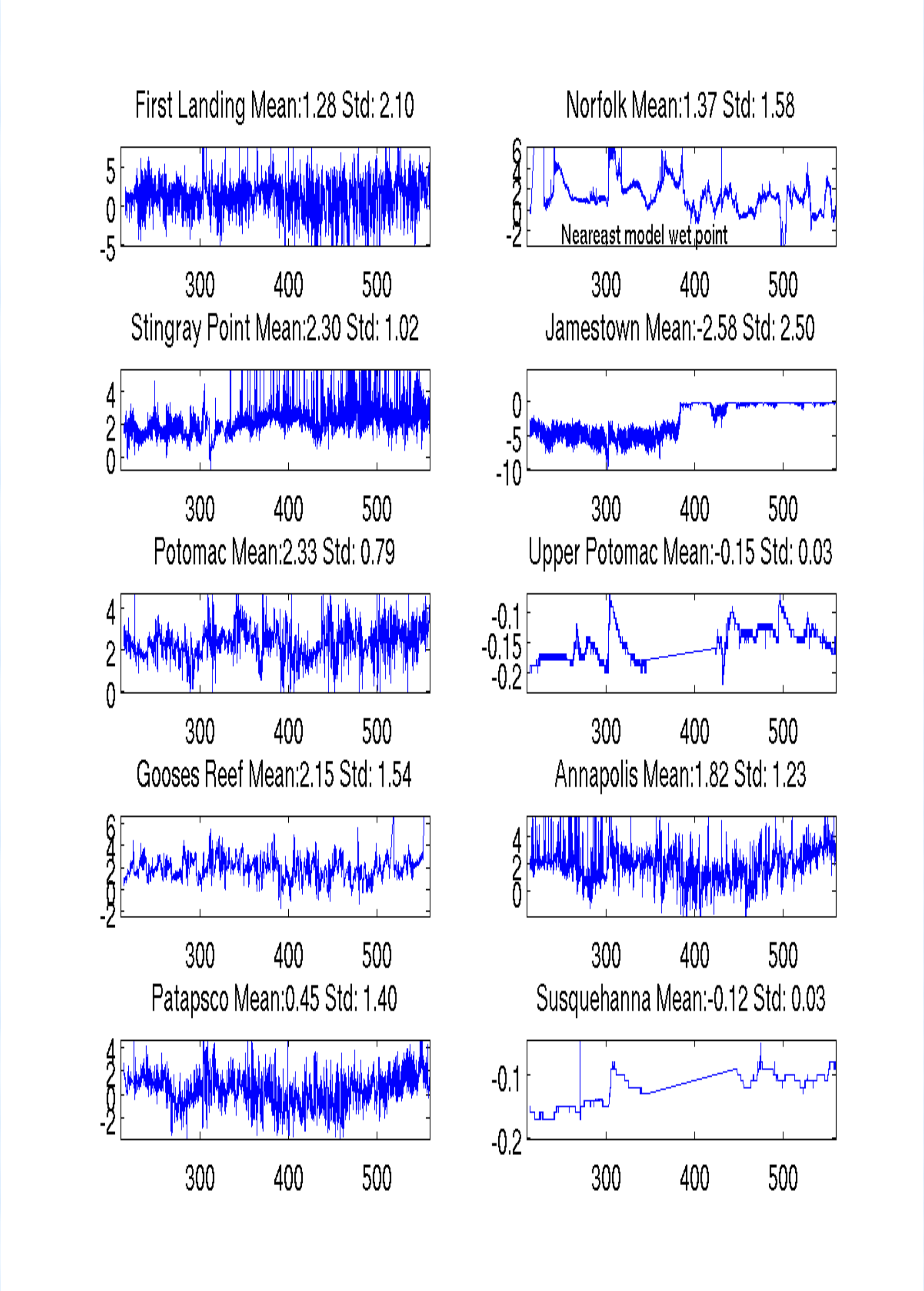
! 1(W) 2(S) 3(E) 4(N)
LBC(isFsur) ==Clo Cla Cha Clo
LBC(isUbar) ==Clo Red Fla Clo
LBC(isVbar) ==Clo Red Fla Clo
LBC(isUvel) ==Clo Rad Rad Clo
LBC(isVvel) ==Clo Rad Rad Clo
LBC(isMtke) ==Clo Gra Gra Clo
LBC(isTvar) ==Clo RadNud RadNud Clo
Clo RadNud RadNud Clo

CBIBS Vs CBOFS (Difference: model-obs)

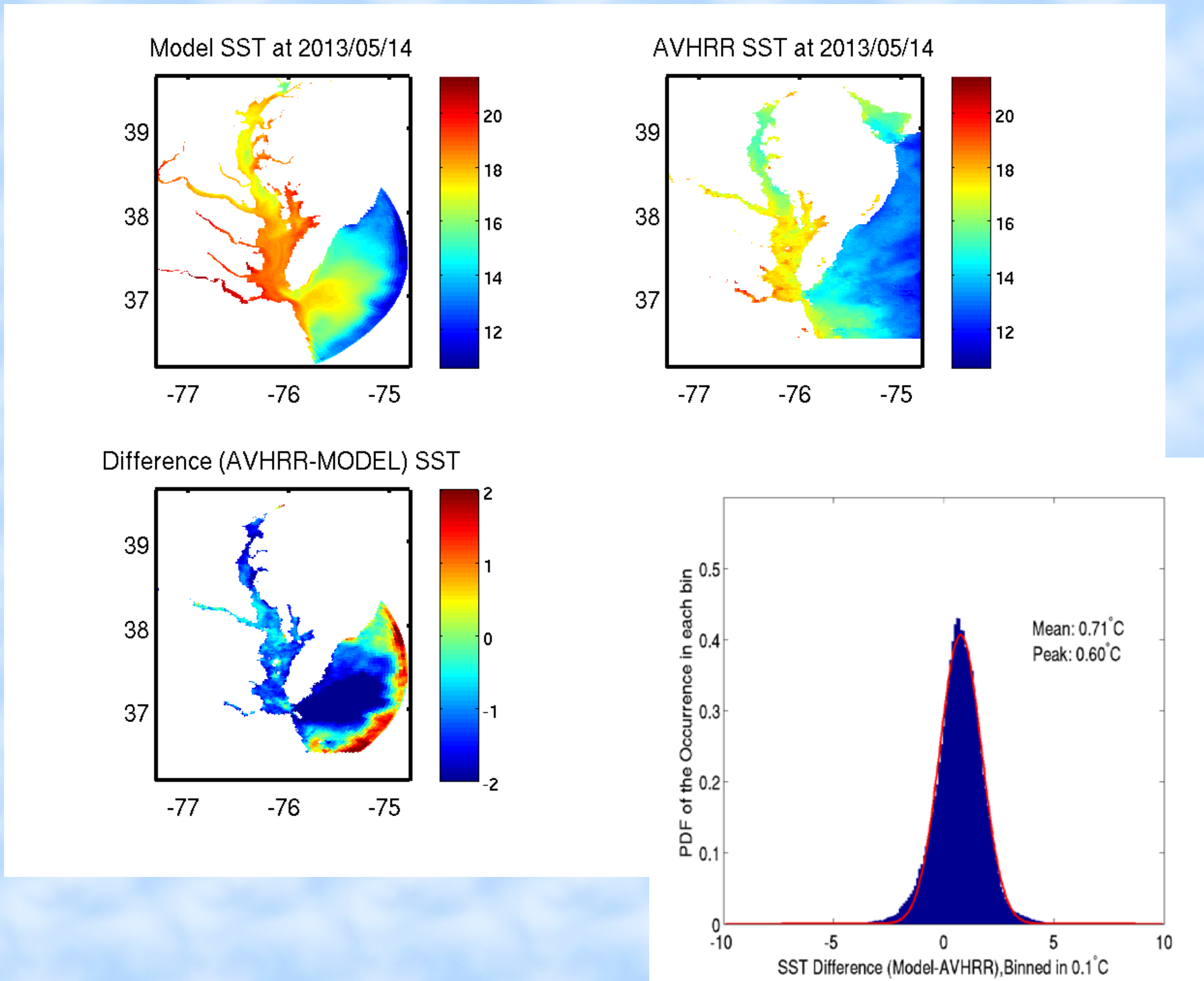
Surface Temperature Difference



Surface Salinity Difference



CBOFS Comparison with Observations



AVHRR SST is from NOAA coastal watch daily composite.

Correlation Matrix C

- Solve a heat diffusion Equations to get C in $[0,\tau_d]$

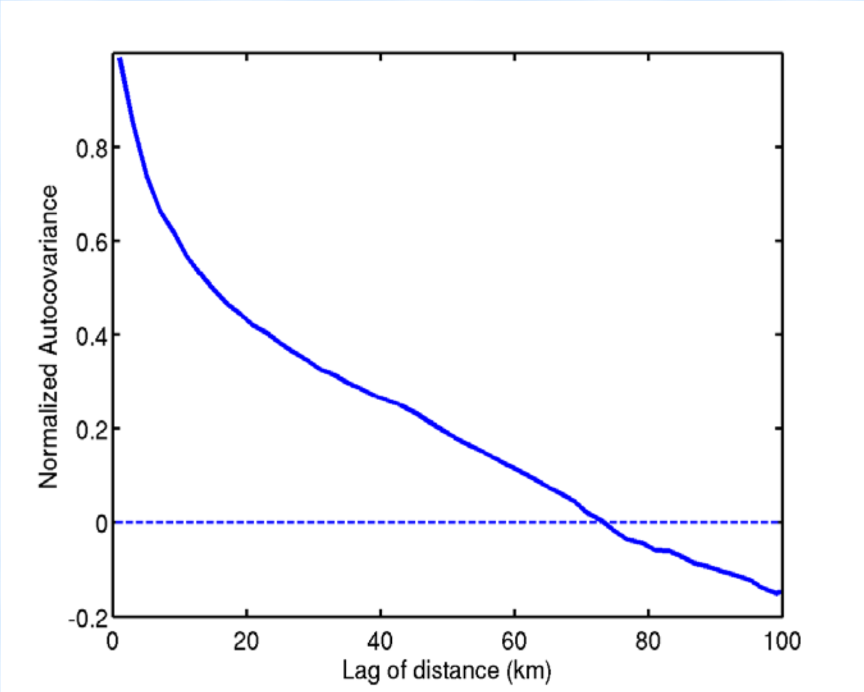
$$\partial\phi/\partial\tau=\kappa\nabla^2\phi\cdots\quad \phi(\tau)=(4\pi\kappa\tau)^{-1/2}C\phi(0)$$

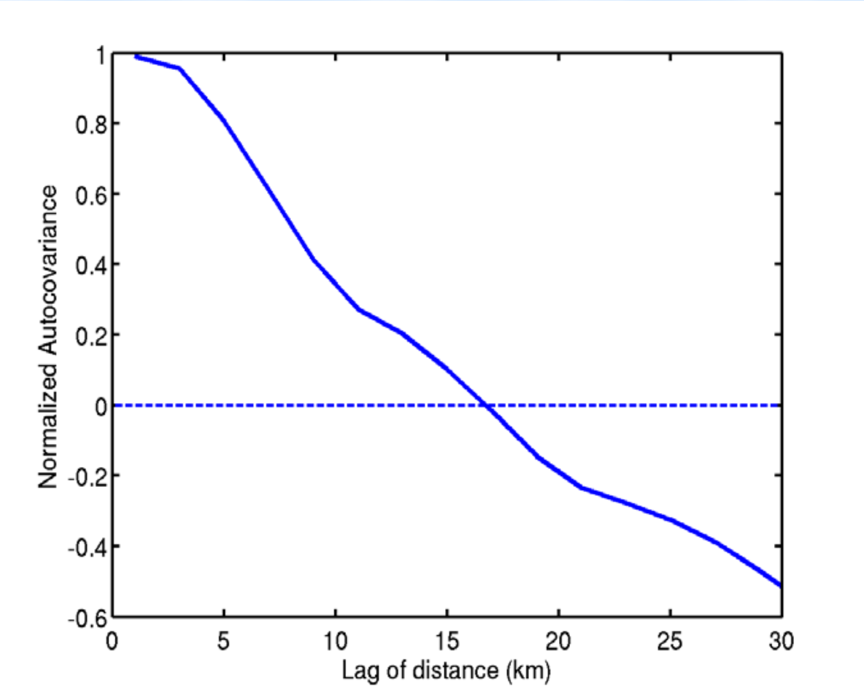
- $L^2=2\pi\tau_d$ Correlation length scale
- Further Decompose C

$$C=\Lambda_h L_h^{\frac{1}{2}} W_h^{-1}(L_h^{\frac{1}{2}})^T \Lambda_h^T$$

- Range of C is in [-1,1], and Λ is the Normalized Coefficient Matrix, W is the model grid area (Moore et al. 2011).
- ROMS Normalization routine saves Λ as output and use it in 4DVAR (exact and random method).

Decorrelation Scales (from SST)





Overall: 73Km

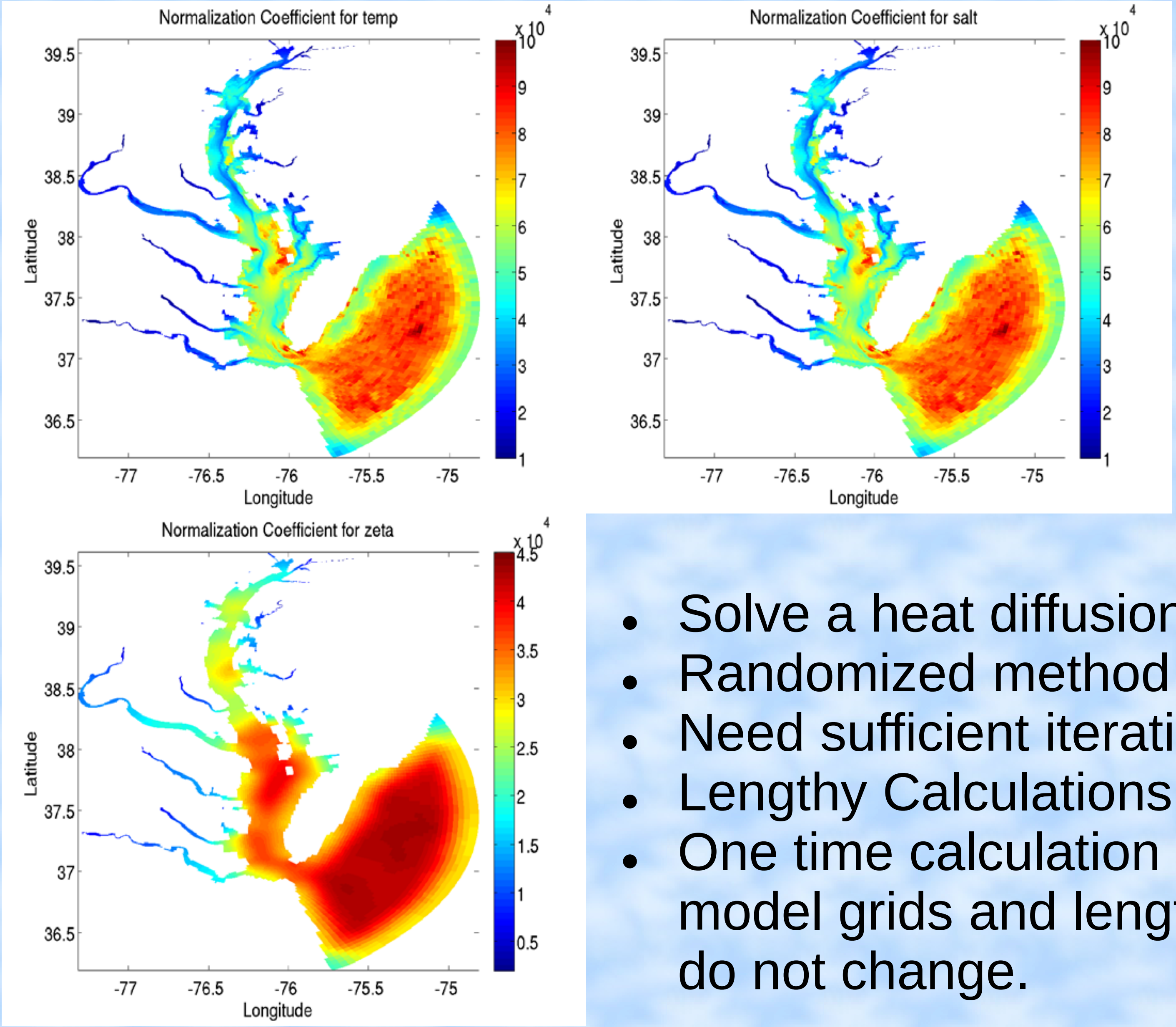
East Direction: 17Km

Autocorrelation

In the vertical, it is hard to get a statistically meaningful decorrelation scale with the shallow depth, we just choose the minimum vertical mixed layer depth to avoid over smoothing. Here we choose it to be 3 m. The surface mixed layer depth ranges from 3m -10m

Ref: http://aslo.org/meetings/santafe1999/abstracts/CS57FR0900E.html

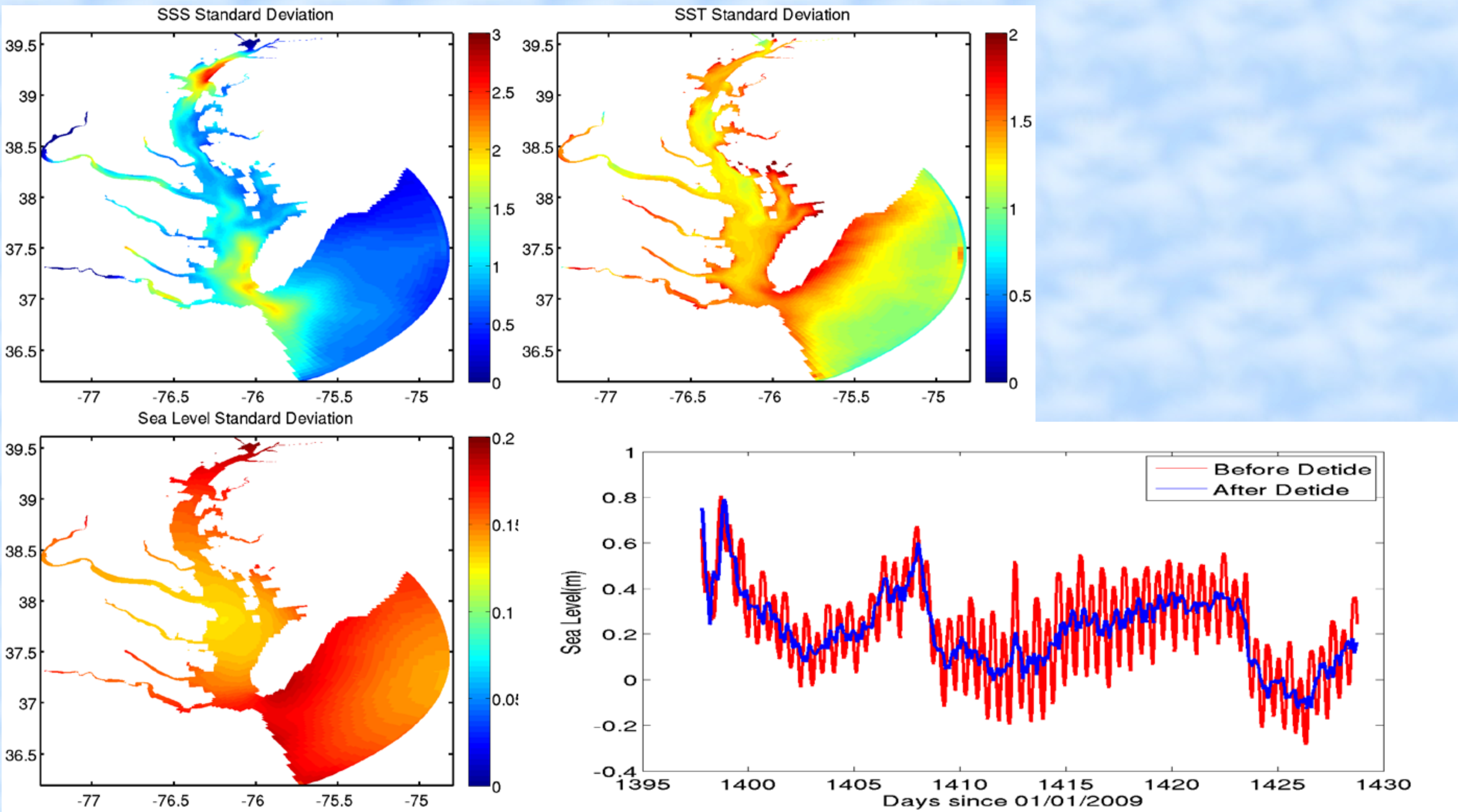
Normalization Coefficients



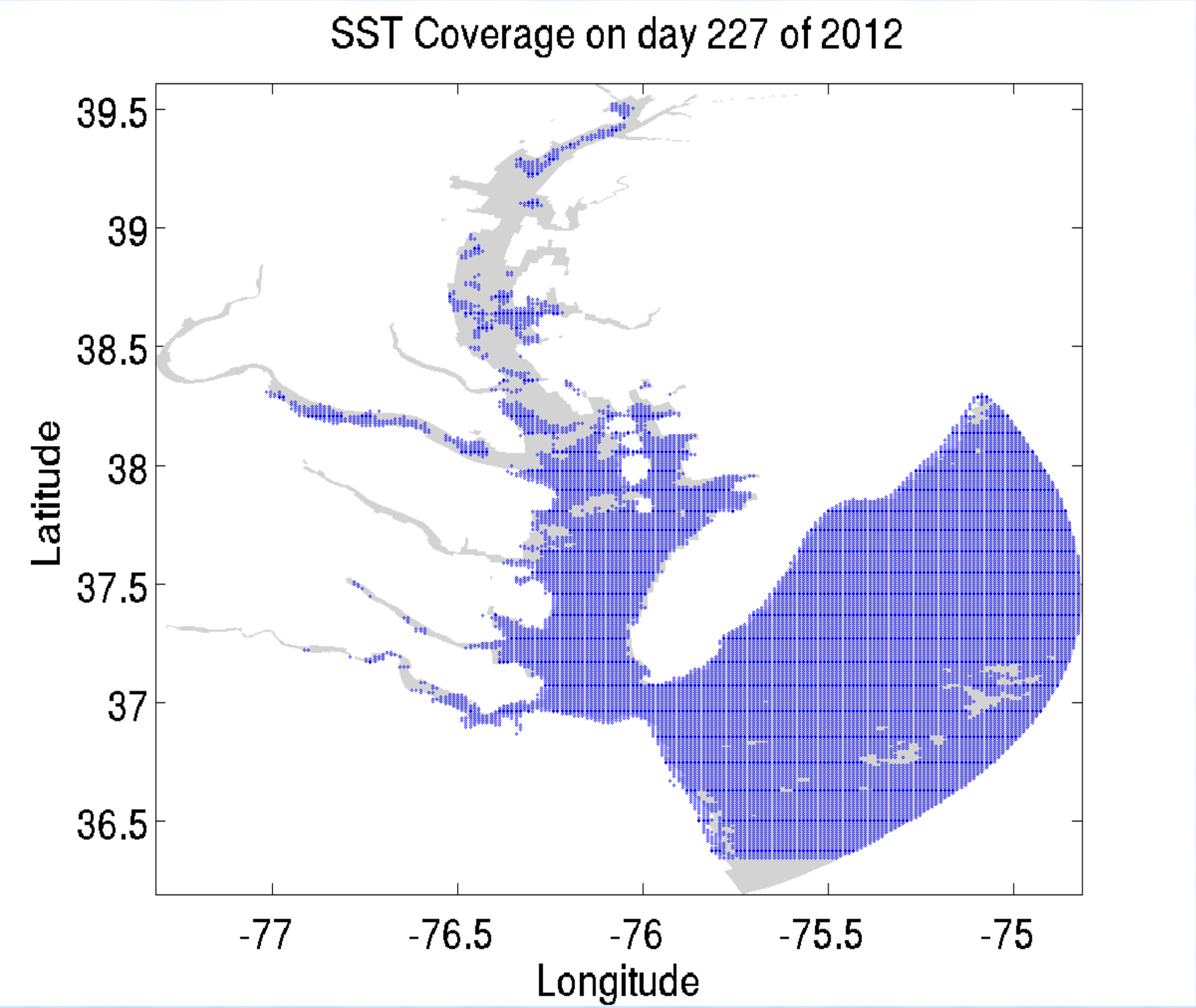
- Solve a heat diffusion equation
- Randomized method
- Need sufficient iterations.
- Lengthy Calculations
- One time calculation if the model grids and length scales do not change.

(Background) Standard Deviation

- Model hindcast for one year, save data with three hours interval.
- Inline least square analysis to calculate tidal harmonics for (T,S,u,v,η).
- Remove periodical signals in the three hourly data (tides and annual signal), and calculate the standard deviation.



SST Observational Matrix



Convert observational lon/lat to I/J index in CBOFS

File Edit View Search Terminal Help

Observational netcdf file

```
netcdf cbofs_sst_obs {
dimensions:
        survey = 3 ;
        state_variable = 7 ;
        datum = 58998 ;
variables:
        int spherical ;
                spherical:long_name = "grid type logical switch" ;
                spherical:flag_values = 0, 1 ;
                spherical:flag_meanings = "Cartesian spherical" ;
        int Nobs(survey) ;
                Nobs:long_name = "number of observations with the same survey time" ;
        double survey_time(survey) ;
                survey_time:long_name = "survey time" ;
                survey_time:units = "days since 2009-01-01 00:00:00" ;
                survey_time:calendar = "gregorian" ;
        double obs_variance(state_variable) ;
                obs_variance:long_name = "global temporal and spatial observation variance" ;
        int obs_type(datum) ;
                obs_type:long = "model state variable associated with observations" ;
                obs_type:flag_values = 1, 2, 3, 4, 5, 6, 7 ;
                obs_type:flag_meanings = "zeta ubar vbar u v temperature salinity" ;
        int obs_provenance(datum) ;
                obs_provenance:long_name = "observation origin" ;
                obs_provenance:flag_values = -1, 1, 2, 3, 4, 5, 6, 7, 8, 9 ;
                obs_provenance:flag_meanings = "gridded_AVHRR_SST_from_NOAA_COASTAL_WATCH gridded_VIIRS_SST_fro
m_NOAA Temperature_from_Chesapeake_Bay_Program Salinity_from_Chesapeake_Bay_Program Temperature_from_Chesapeake
_Bay_Interactive_Buoy_System Salinity_from_Chesapeake_Bay_Interactive_Buoy_System Temperature_from_USGS_river_n
etwork_ Salinity_from_USGS_river_network u_velocity_(ROMS_u)_from_Old_Dominion_HF_Radar v_velocity_(ROMS_v)_fro
m_Old_Dominion_HF_radar" ;
        double obs_time(datum) ;
                obs_time:long_name = "time of observation" ;
                obs_time:units = "days since 2009-01-01 00:00:00" ;
                obs_time:calendar = "gregorian" ;
        double obs_lon(datum) ;
                obs_lon:long_name = "observation longitude" ;
                obs_lon:units = "degrees_east" ;
                obs_lon:standard_name = "longitude" ;
        double obs_lat(datum) ;
                obs_lat:long_name = "observation latitude" ;
                obs_lat:units = "degrees_north" ;
                obs_lat:standard_name = "latitude" ;
        double obs_depth(datum) ;
                obs_depth:long_name = "depth of observation" ;
                obs_depth:units = "meters" ;
                obs_depth:negative = "downwards" ;
        double obs_Xgrid(datum) ;
                obs_Xgrid:long_name = "observation fractional x-grid location" ;
        double obs_Ygrid(datum) ;
                obs_Ygrid:long_name = "observation fractional y-grid location" ;
        double obs_Zgrid(datum) ;
                obs_Zgrid:long_name = "observation fractional z-grid location" ;
        double obs_error(datum) ;
                obs_error:long_name = "observation error covariance" ;
        double obs_value(datum) ;
                obs_value:long_name = "observation value" ;
--More--
```

IS4DVAR ROMS Setup

CPP Options

```
#define IS4DVAR
#define CBOFS
#ifdef IS4DVAR
# define ADJUST_BOUNDARY
# define ADJUST_WSTRESS
# define ADJUST_STFLUX
# define FORWARD_MIXING
# define FORWARD_READ
# define FORWARD_WRITE
# define VCONVOLUTION
# define IMPLICIT_VCONV
#endif
#define  ATM_PRESS
#OTHER CPP options
```

Adjoint Boundary Conditions are different from Nonlinear model.

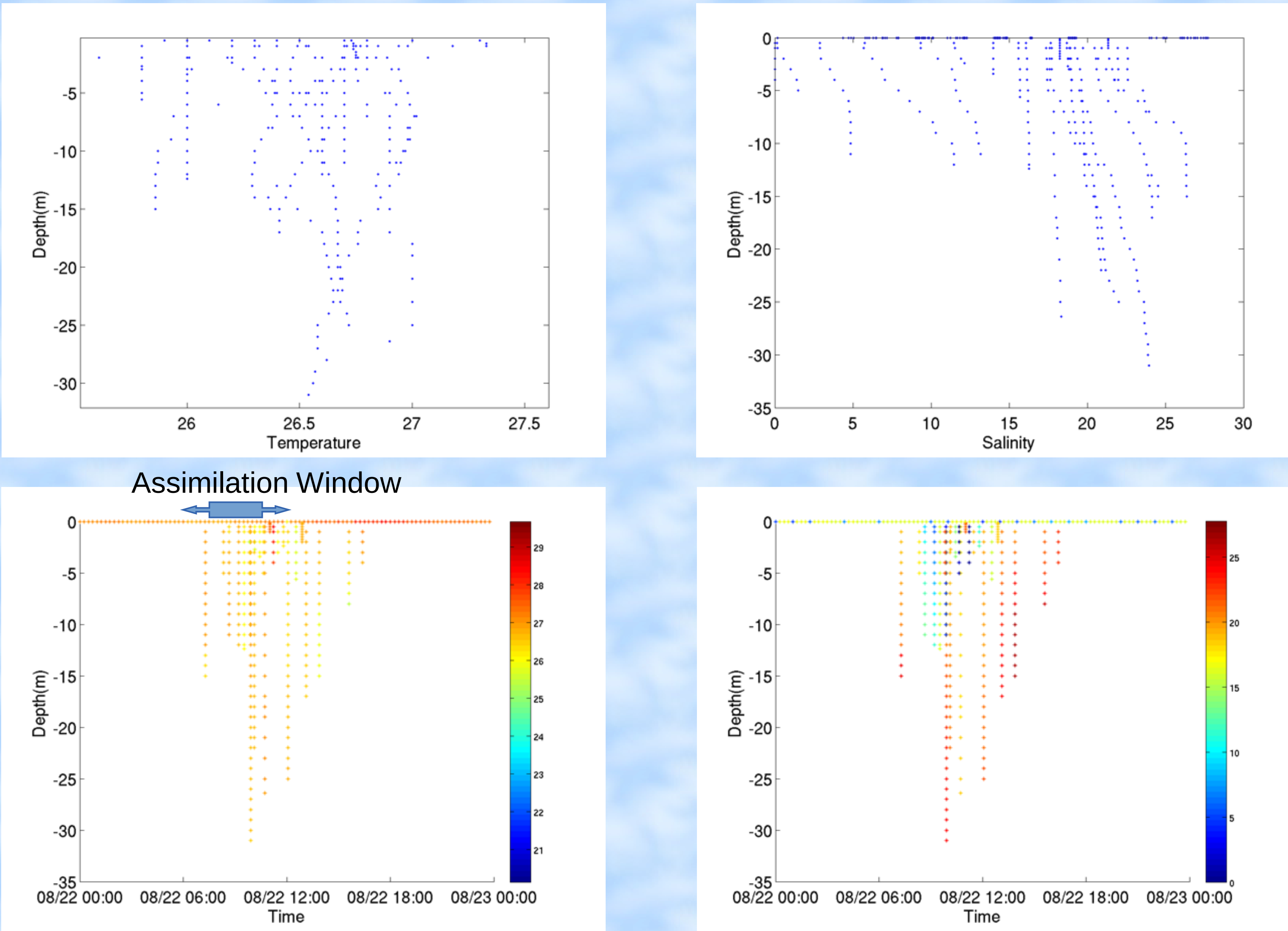
	W	S	E	N
ad_LBC(isFsur) ==	Clo	Clo	Clo	Clo
ad_LBC(isUbar) ==	Clo	Red	Fla	Clo
ad_LBC(isVbar) ==	Clo	Red	Fla	Clo
ad_LBC(isUvel) ==	Clo	Gra	Gra	Clo
ad_LBC(isVvel) ==	Clo	Gra	Gra	Clo
ad_LBC(isMtke) ==	Clo	Gra	Gra	Clo

```
ad_LBC(isTvar) ==   Clo   Cla   Cla   Clo \
                    Clo   Cla   Cla   Clo
```

Preconditioning is set:
Ritz Limited-Memory Preconditioner

Assimilation with T/S Profiler data

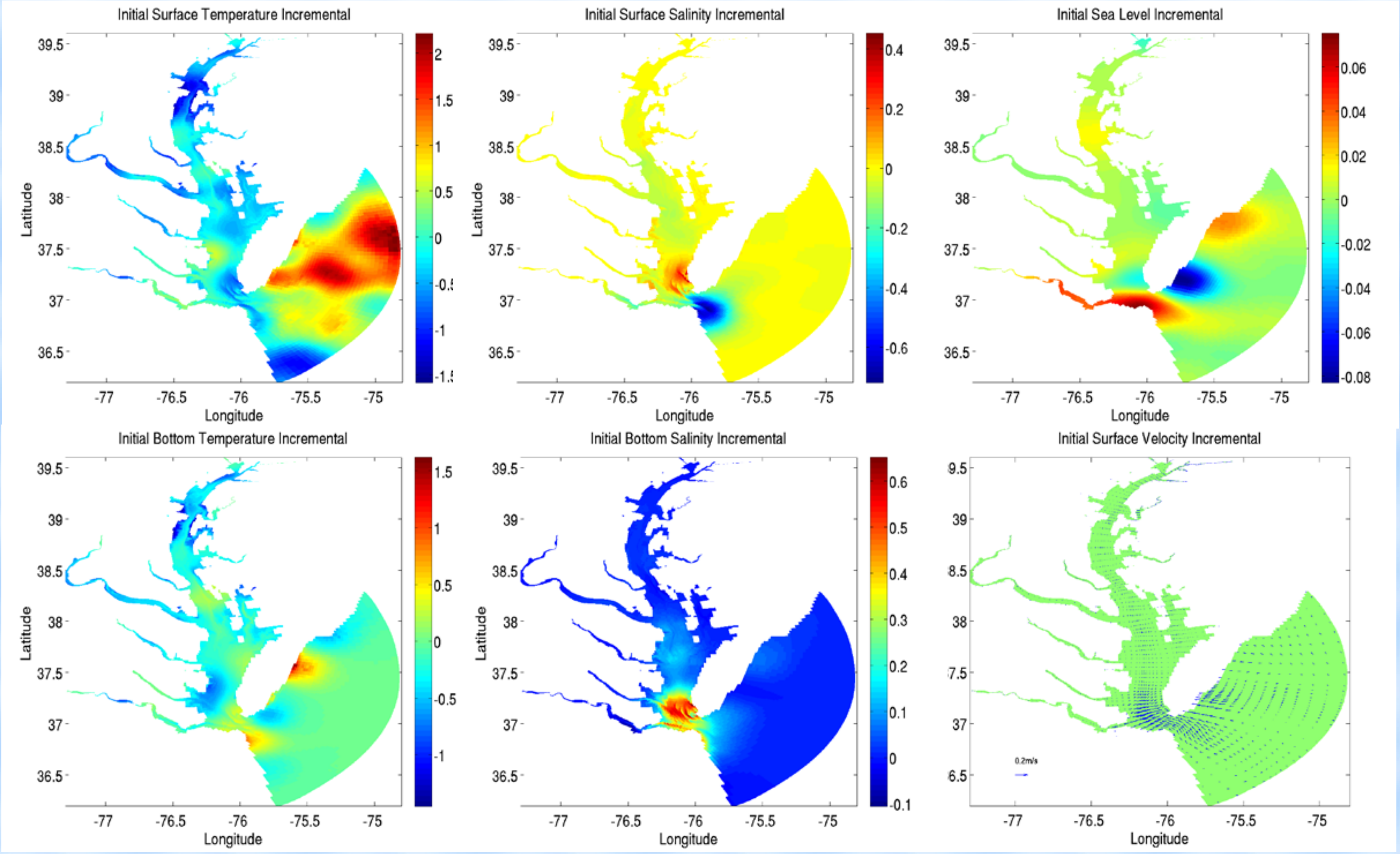
Observational Data at CBIBS (surface) and CBP (Profiler)



Temperature Salinity

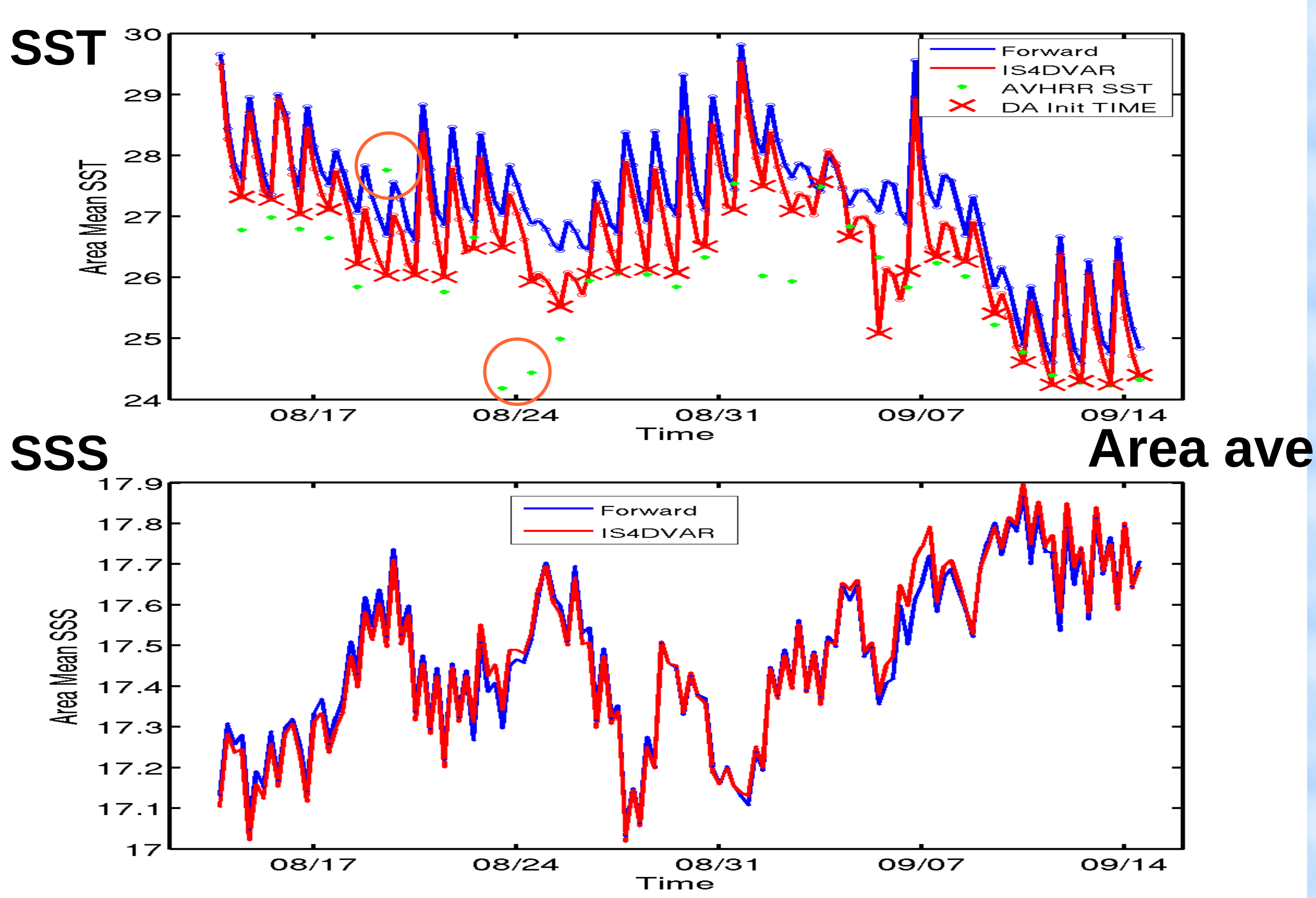
IS4DVAR (Incrementals)

Initial Condition Difference before and after IS4DVAR. 08/15/2012 12:00



The temperature is modified by SST assimilation but salinity and velocity changes mostly in the Chesapeake Bay mouth region. The adjustment of salinity and velocity in the mouth area is more sensitive to the SST than other area.

One month Sequential Adjustment of Initial Condition with AVHRR SST

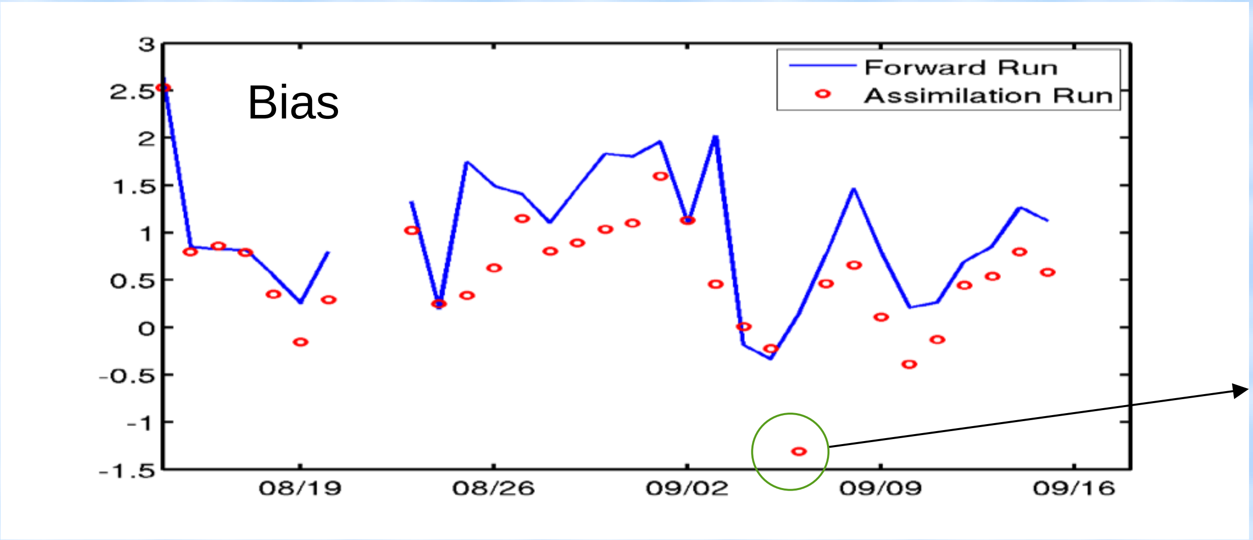


Area averaged

Mean FWD SST: 27.25 Mean DA SST: 26.74; Mean FWD SSS: 17.469;
Mean Sat SST: 25.89 Mean DA SSS: 17.467;

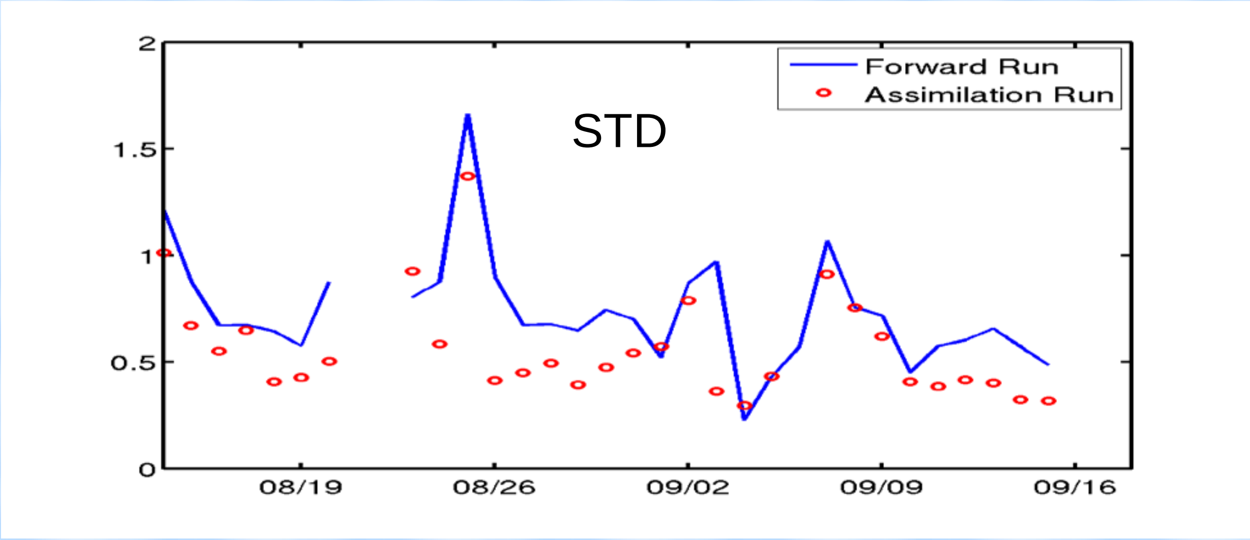
Comparison with observations (AVHRR)

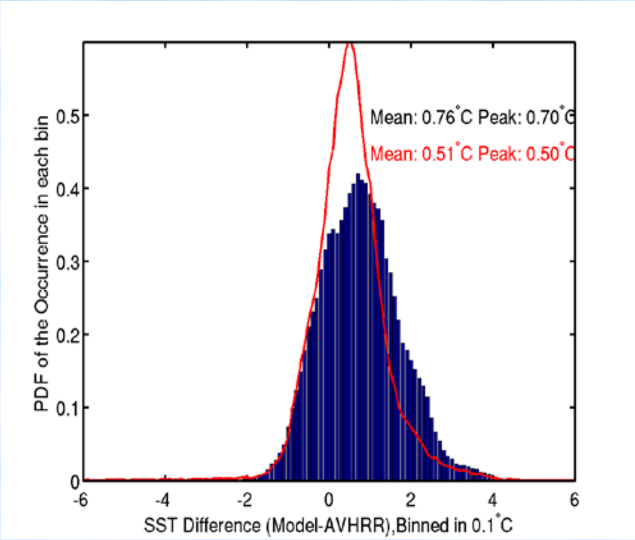
Difference between model and observations
at observational location



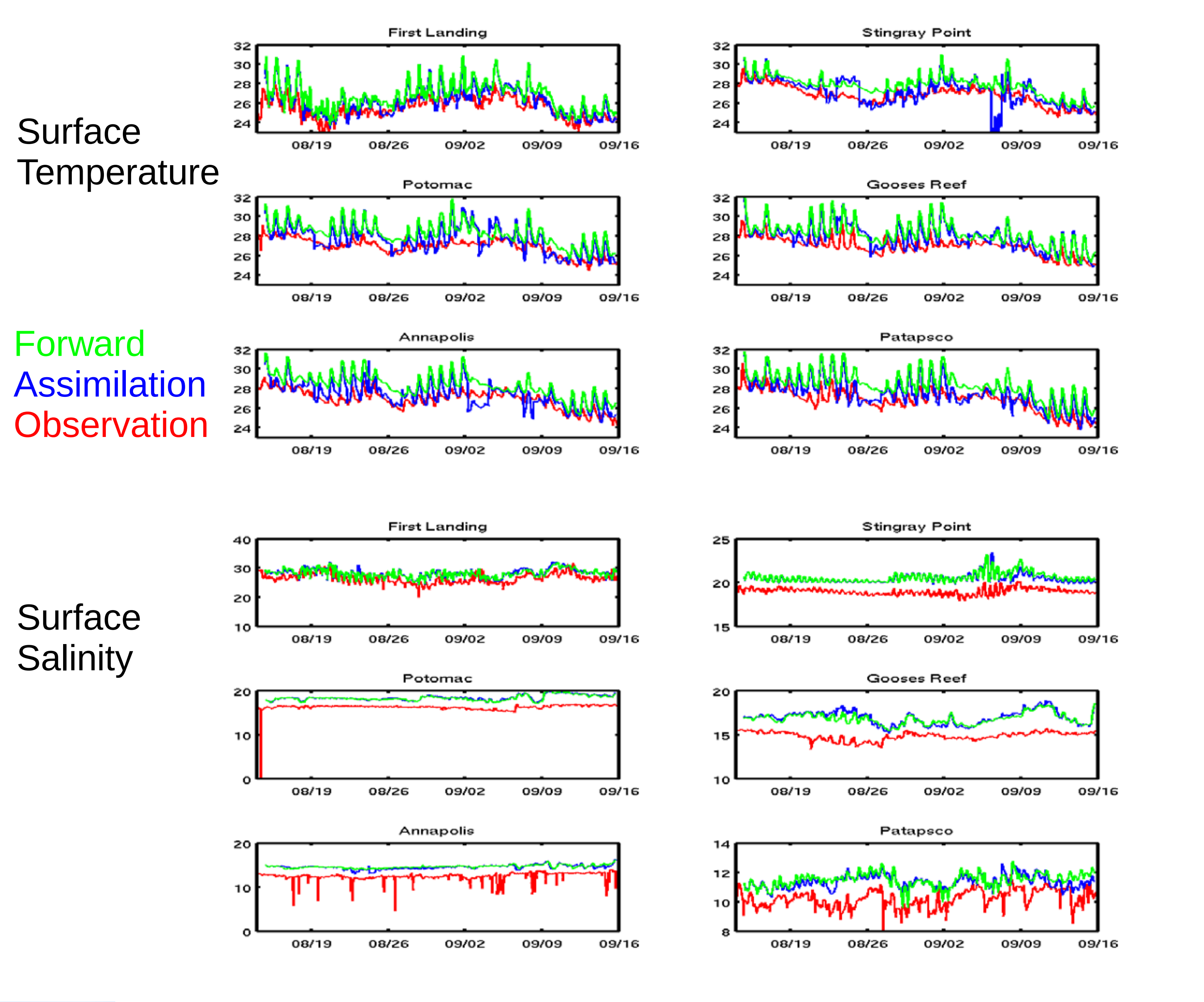
Total bias reduction: 0.45 Deg_C and Standard deviation of difference also reduced by 0.1

A few low SST values are assimilated here.

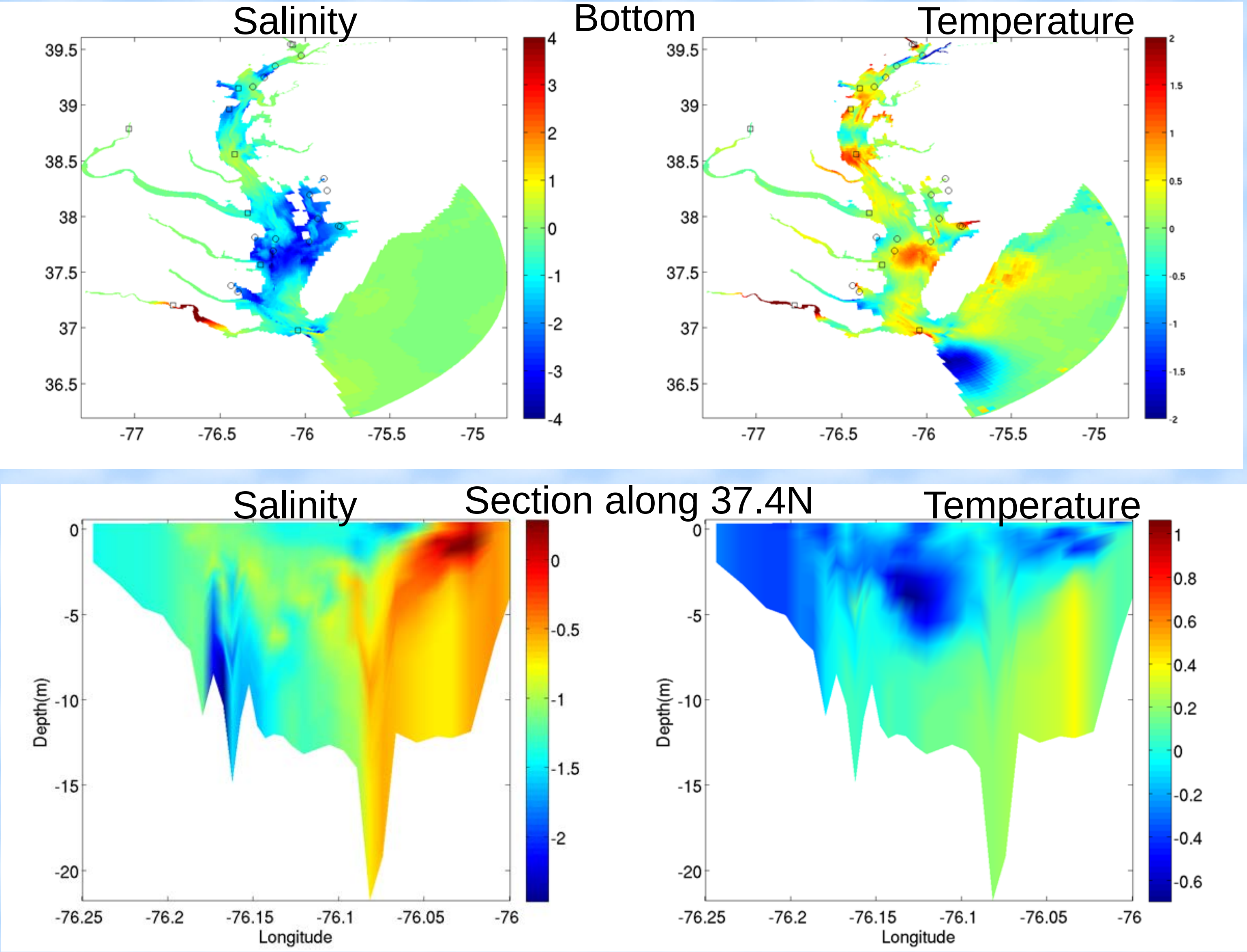




Comparison with observations (CBIBS)



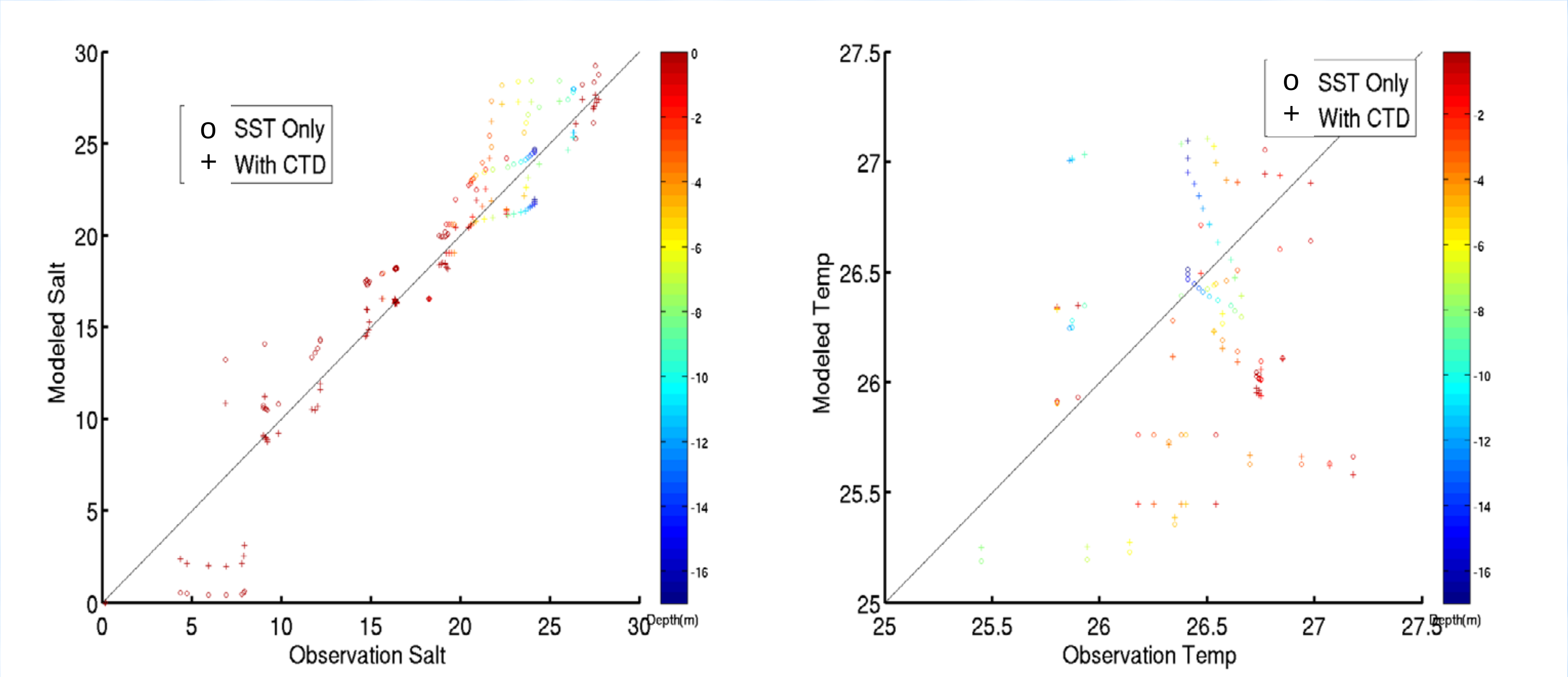
Salt/Temp Changes



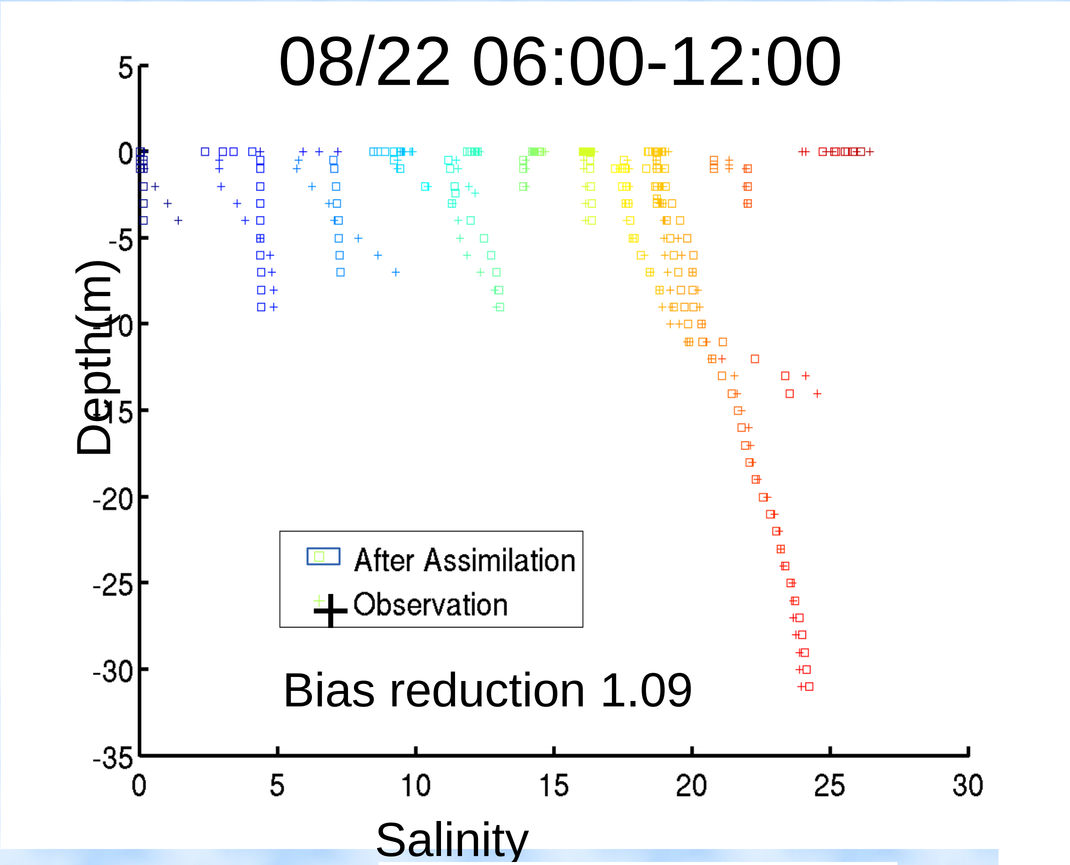
Temperature and salinity difference of model runs with and without assimilation of CBP and CBIBS temperature and salinity observations at 18:00 22 August 2012 along a transect 37.41ºN. Both cases are assimilated with AVHRR SST.

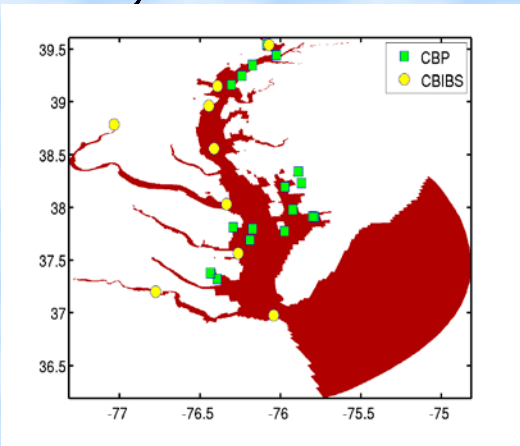
Validation using unassimilated data at forecasting window

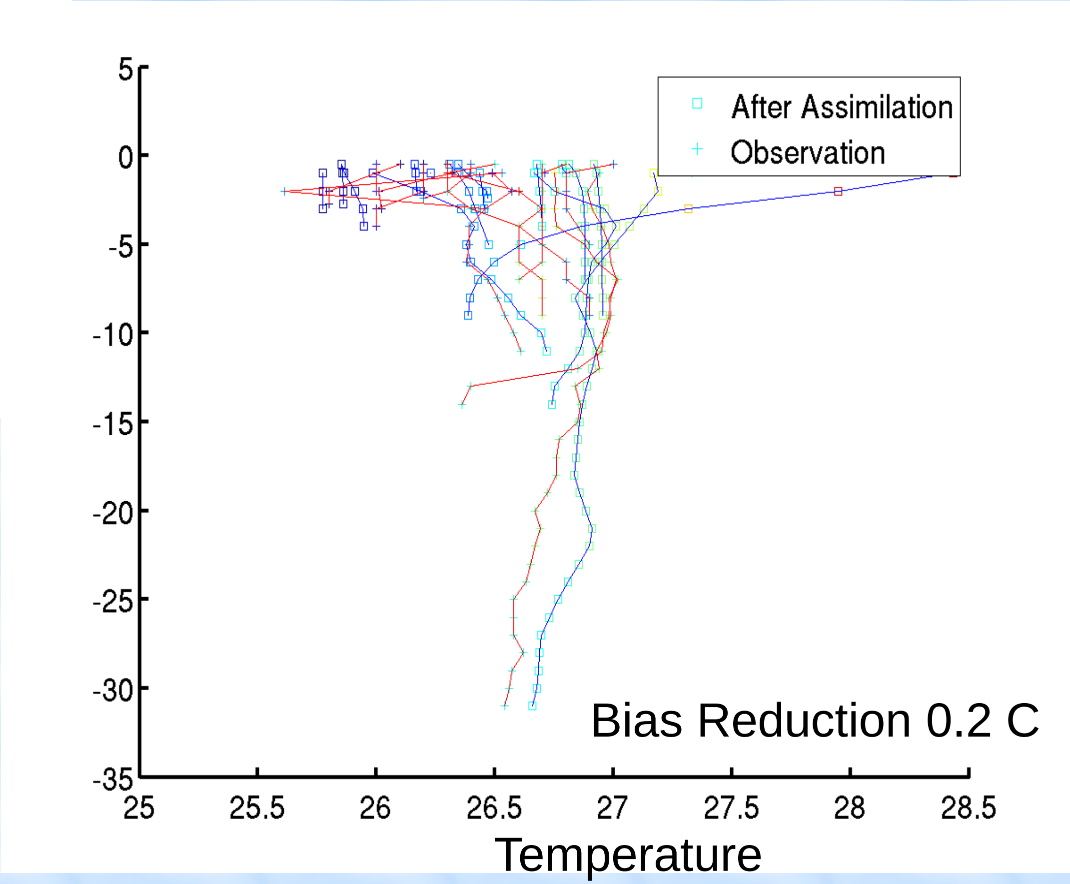
08/22 12:00-18:00



Assimilation with T/S data







FWD/IS4DVAR vs VIIRS SST

at CBIBS locations

VIIRS SST-IS4DVAR SST

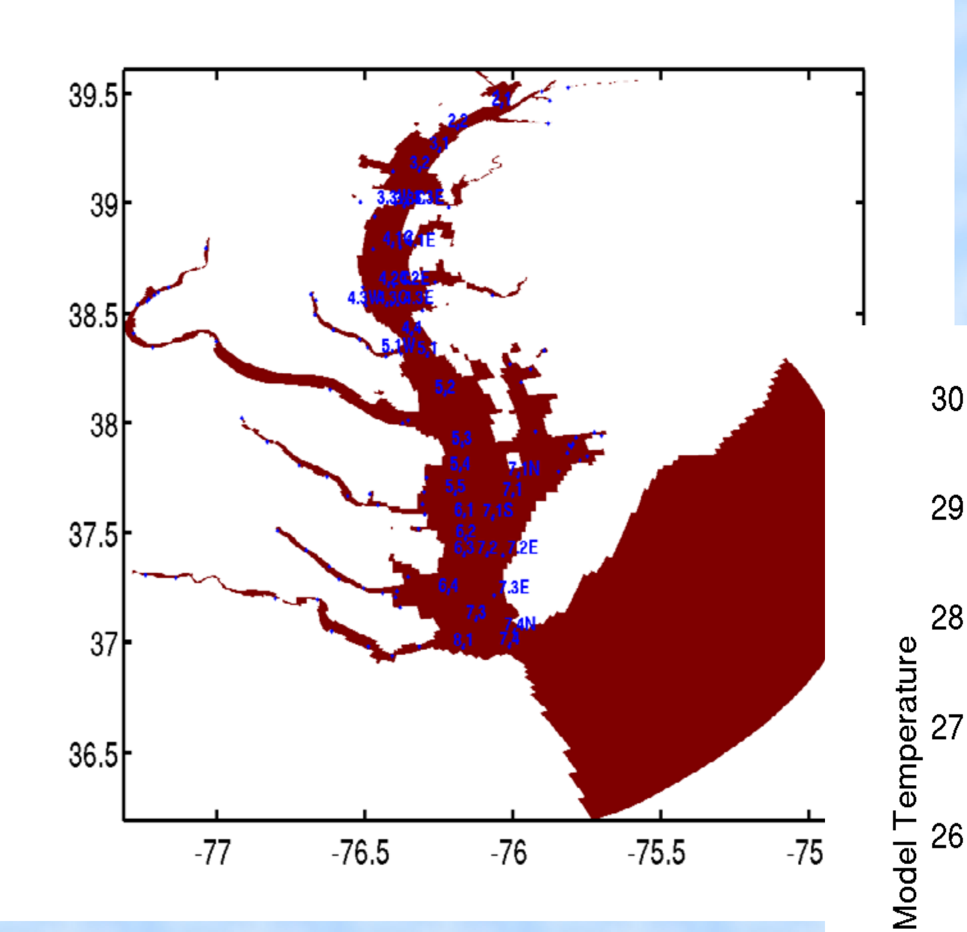
Stations	First Landing	Stringray Point	James town	Potomac	Upper Potomac	Gooses Reef	Annapolis	Patapsco	Susquehan na	RCU
SST Diff	-0.31	-0. 05	-0.32	-0.18	-0.02	-0.27	-0.19	-0.20	0.56	-0.11
SST STD	0.91	0.61	0.60	0.75	0.18	0.92	0.73	0.76	0.72	0.54
TOTAL Number	69	68	17	56	6	75	64	69	40	13

VIIRS SST-FWD SST

at CBIBS locations

Stations	First Landing	Stringray Point	James town	Potomac	Upper Potomac	Gooses Reef	Annapolis	Patapsco	Susquehan na	RCU
SST Diff	-1.40	-0.90	-0.56	-1.16	-0.47	-1.40	-1.37	-1.44	1.41	-0.29
SST STD	1.12	0.81	0.69	0.98	0.77	1.01	0.81	0.82	1.73	0.73
TOTAL Number	173	176	54	163	19	187	153	165	88	26

Comparison with CBP Observations

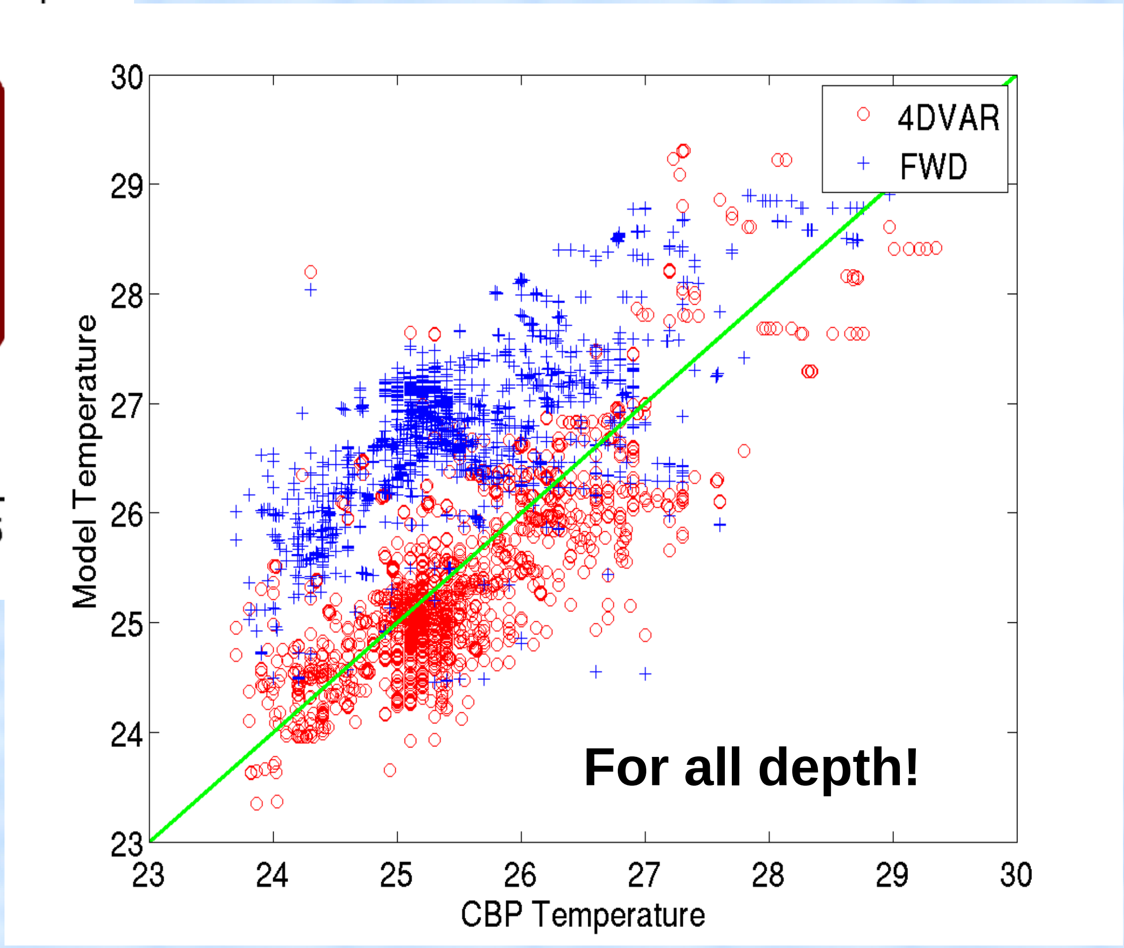


Before:

CBOFS vs CBP: 1.27° C ± 0.70° C

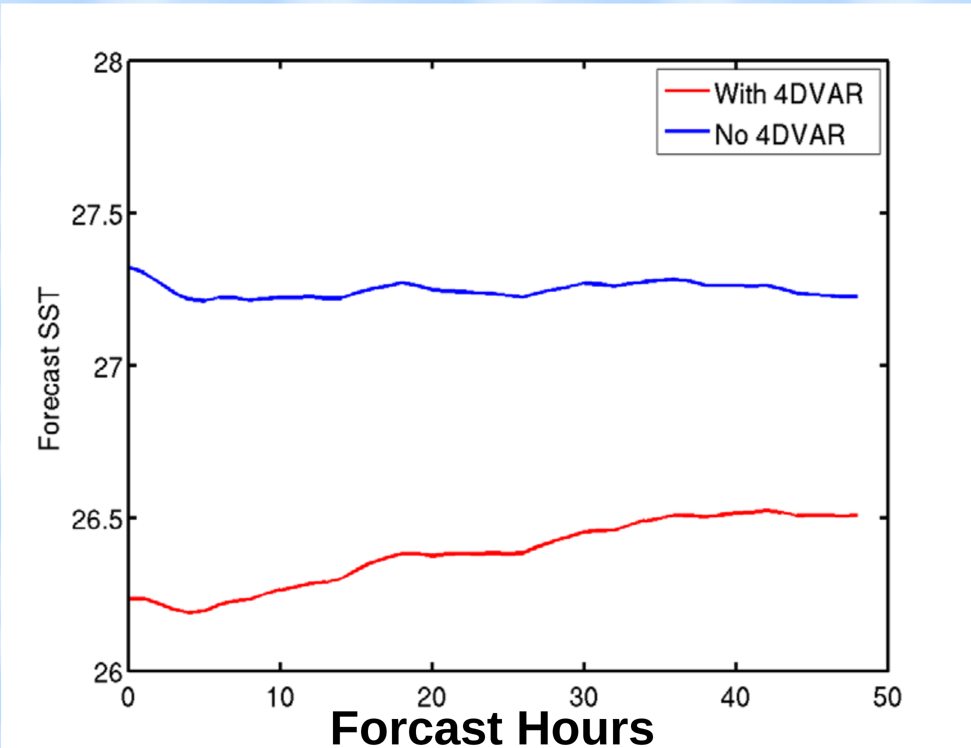
After:

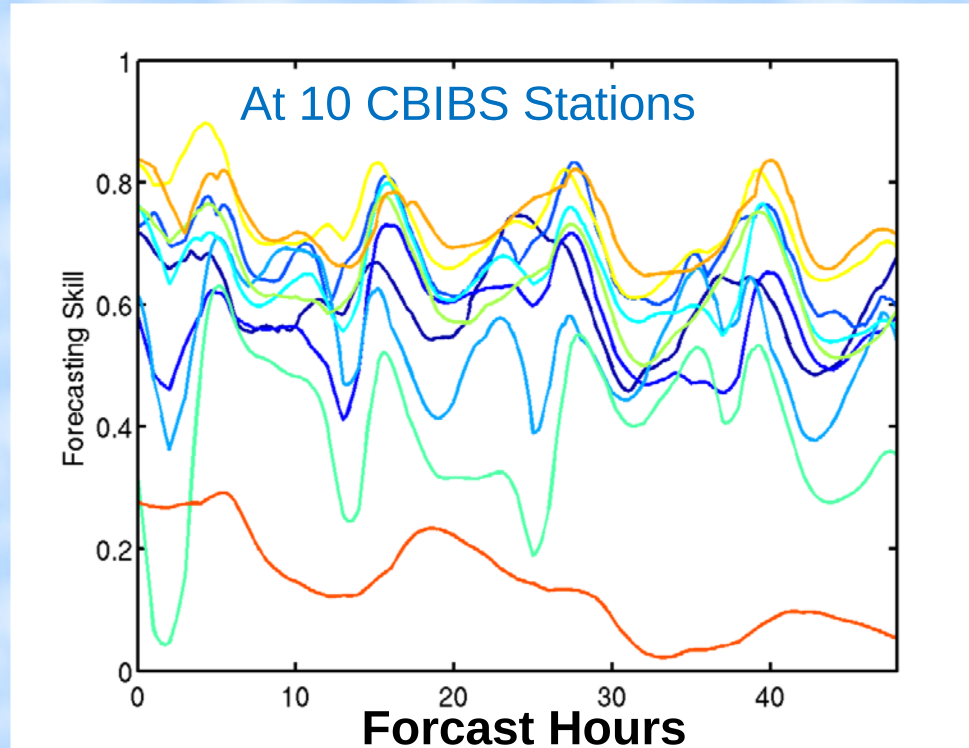
I4DVAR vs CBP: -0.08° C ± 0.6° C



Scatter plots of observed temperature at CBP stations vs the 4DVAR temperature and the forward model temperature at all depth.

Forecasting Skills





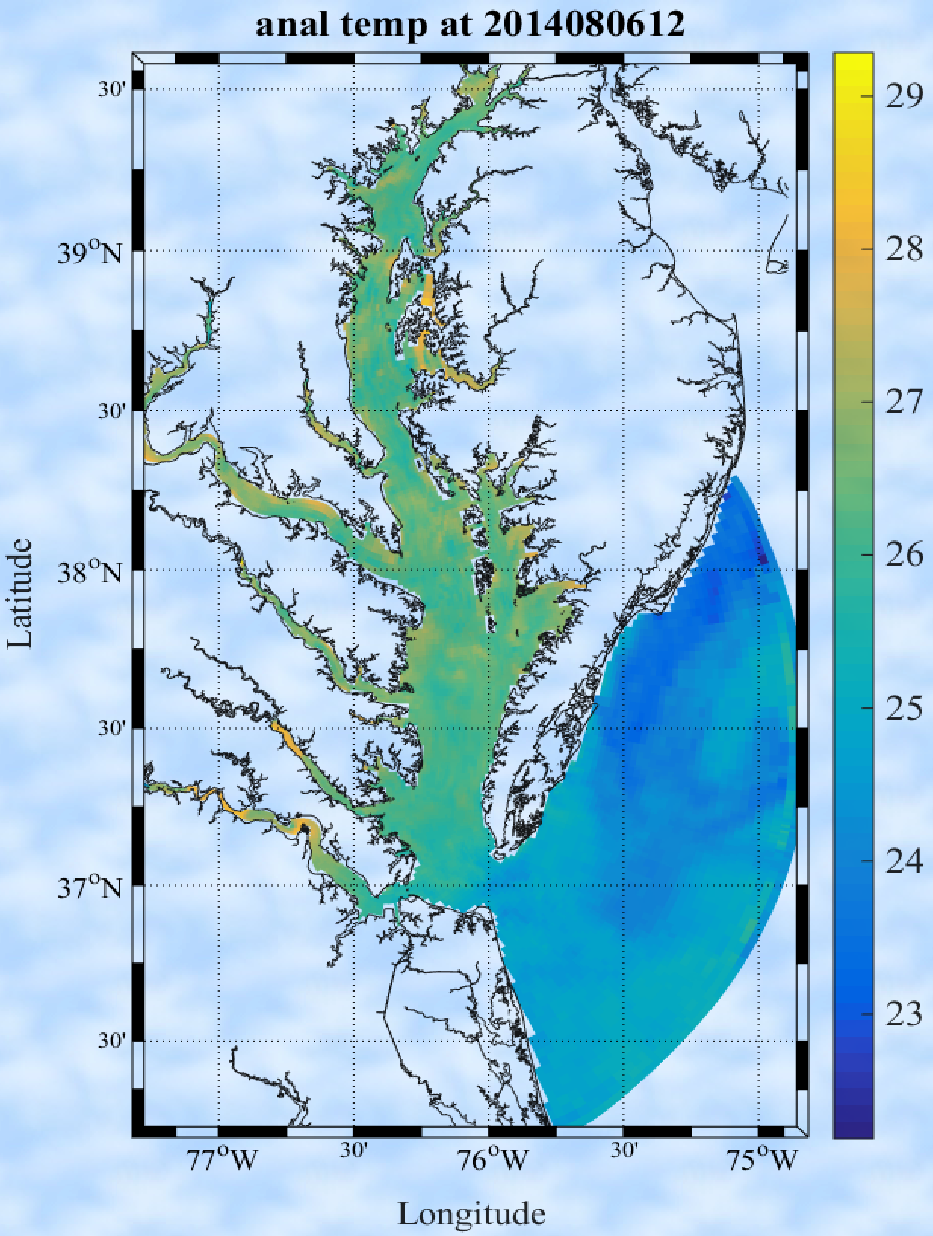
Area mean forecasting SST Reduction

Along with increasing of forecasting time, the forecast SST from new analysis gradually approaches that without DA. Notice the diurnal cycle due to surface Forcing modulation.

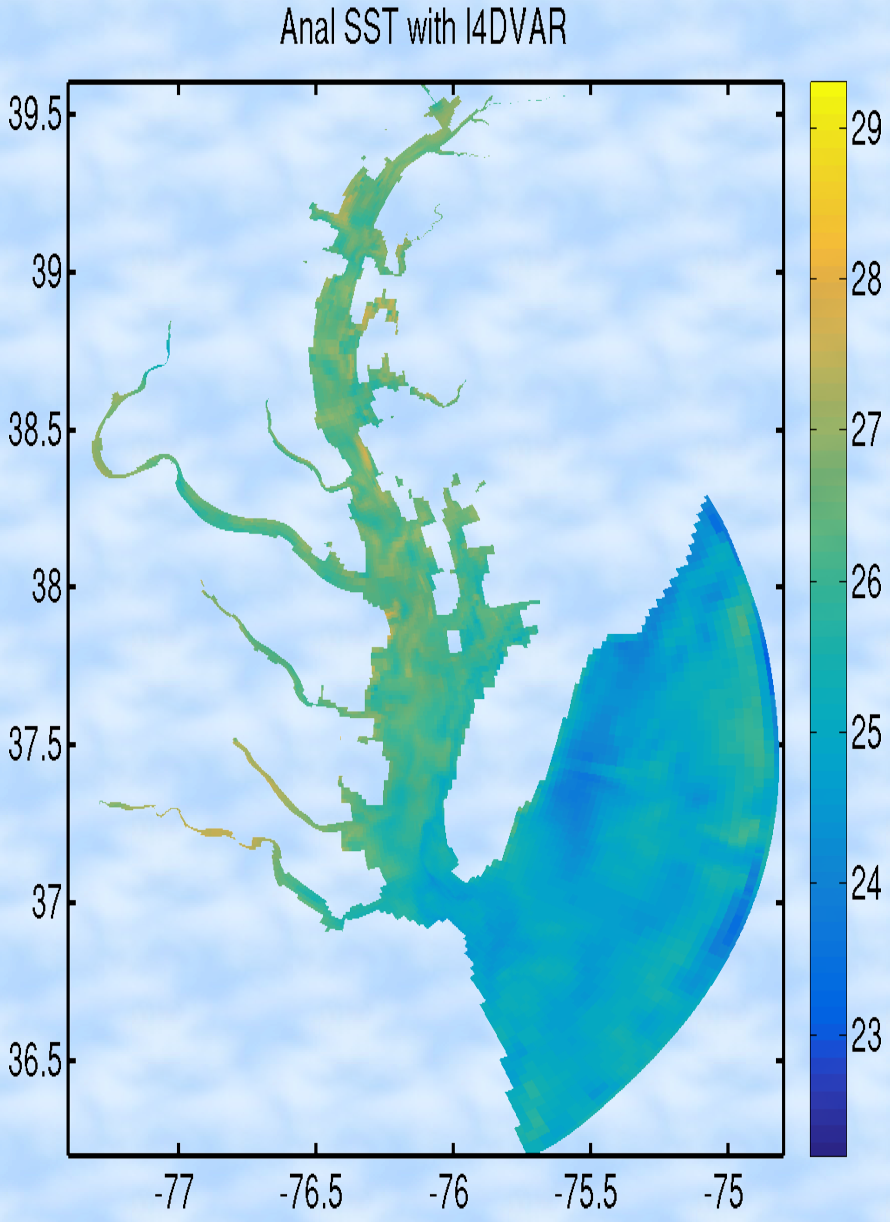
$$\mathbf{S} = 1 - \frac{\sum(F_i^a - O_i)}{\sum(F_i - O_i)}$$

$$\mathbf{S} = \begin{cases} 1, \text{ Perfectly match observations.} \\ 0, \text{ neither improve nor deteriorate.} \\ <0, \text{ less skillful in performance.} \end{cases}$$

Initial Comparison with LETKF



LETFK



4DVAR

Ongoing work

- Keep analyzing VIIRS data assimilation

About three months data assimilation ready from 08/06/2014

- Analysis of AVHRR SST data assimilation

Have one month data assimilation ready from 08/06/2014

- Compare with results from LETKF.
- Paper/Report writing
- Transfer of data assimilation codes into operational mode (regarding the computational cost, performance etc) to CSDL/CO-OPS.

Observational File Creation

- Format : NetCDF

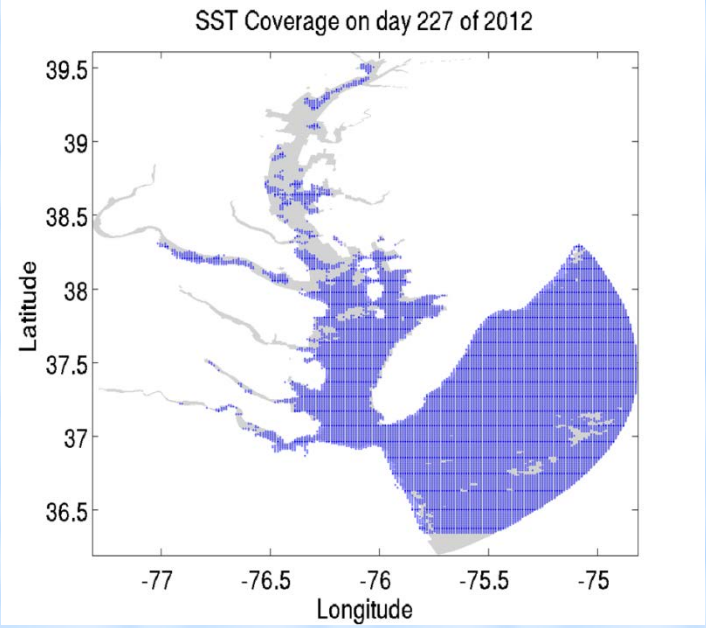
  Observation locations to ROMS grid (Horizontal), and depth;

  Observation time and Survey time (e.g. one CTD casting).

  Observation source (optional: CTD, XBT, SST etc)

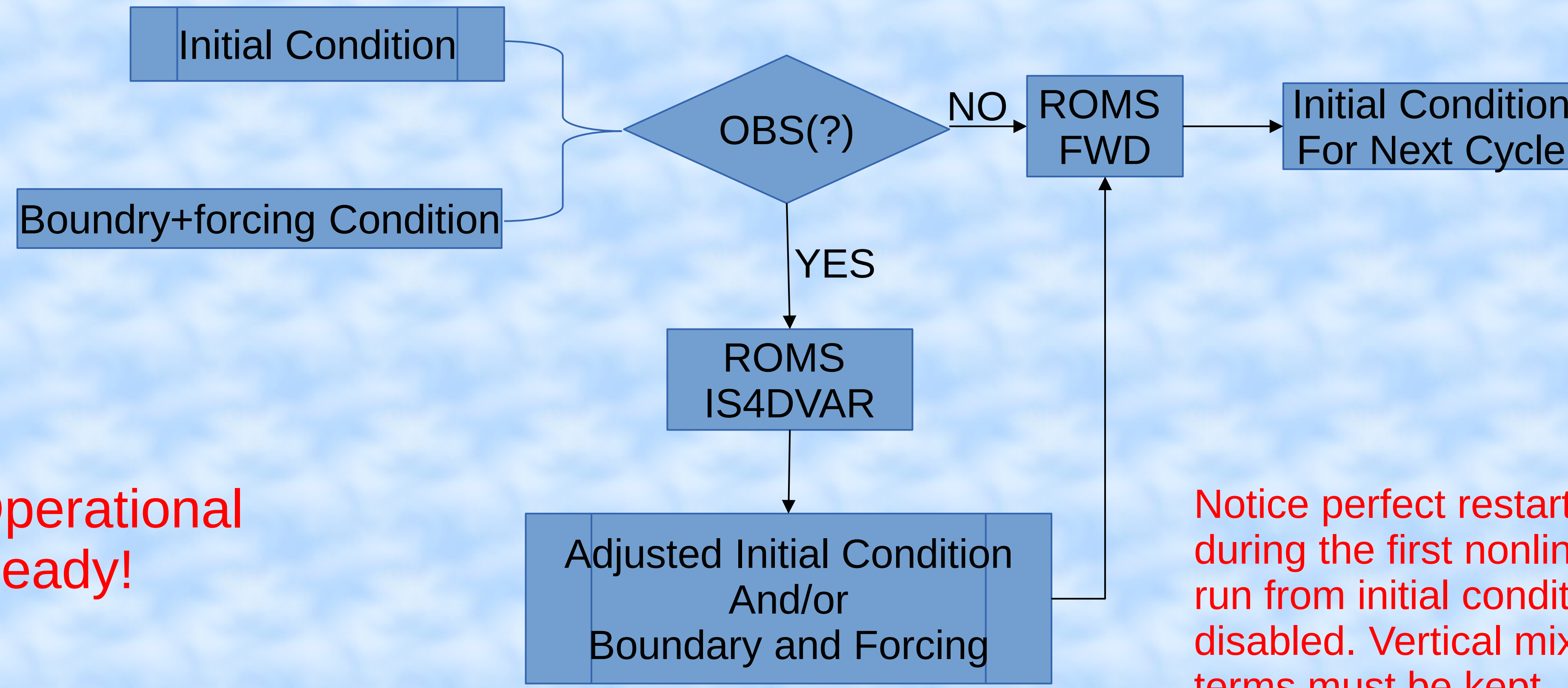
  Observation value and error.

- Coded matlab code for CBOFS, mainly spatial interpolation of VIIRS/AVHRR pixels to CBOFS grids.
- Observational error from SST product
- Spatial averaging in one model grids



Flow Chart for IS4DVAR

Forward Run Window



Operational Ready!

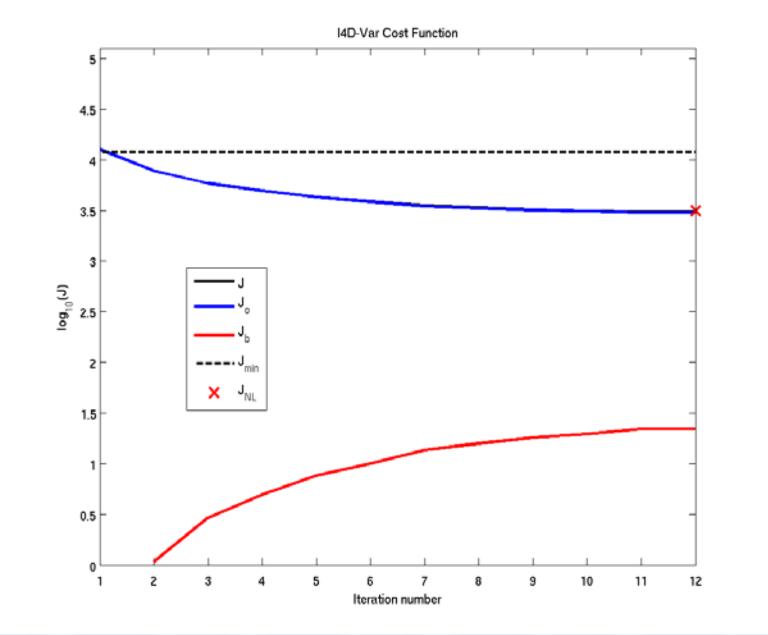
Notice perfect restart during the first nonlinear run from initial condition is disabled. Vertical mixing terms must be kept.

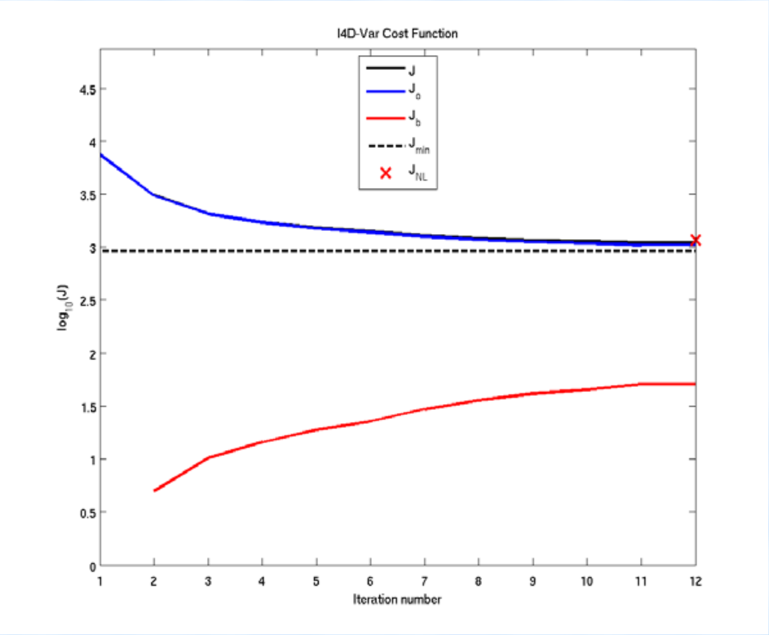
Forward Run Window/Assimilation Window (6 hours)

Sequential run from 08/06/2014 06:00 to 11/06/2014 00:00

A bash script is setup for this.

IS4DVAR Cost Function (Adjustment of Initial Condition only)





08/14/2012 12:00
Nobs=23806

08/23/2012 12:00
Nobs=1817

The total penalty function J decreases to a near-stable number in a 10 inner loops.

4DVAR Computational Load

- Twice assimilation per day usually for VIIRS SST.
- 4DVAR runs were completed using 96 Ivy Bridge 2.8 GHz Processors from deepthought2 at UMD.
- Granted 260k CPU hours for this project from UMD/OIT!

DA Method	Processors	Time to run 6 hours	Time for one 2.8G Hz CPU	Notes
I4DVAR	96 (2.8 GHz)	~6.3 hours	~604 hours	15 inner loops /1 outer loop

Operationally doable!