Ensemble 4DVAR data assimilation in a dynamically challenging coastal ocean environment

IVO PASMANS

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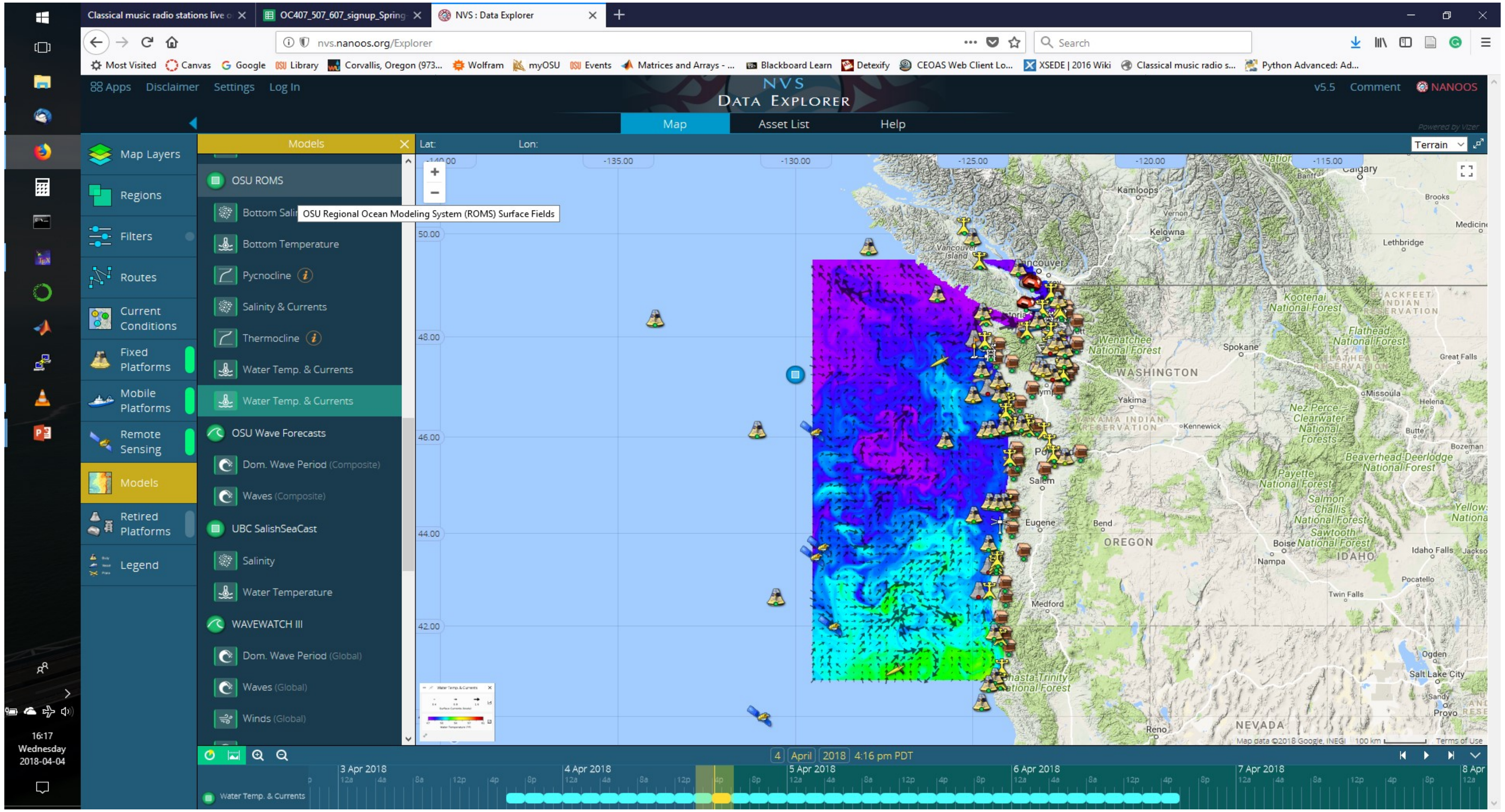
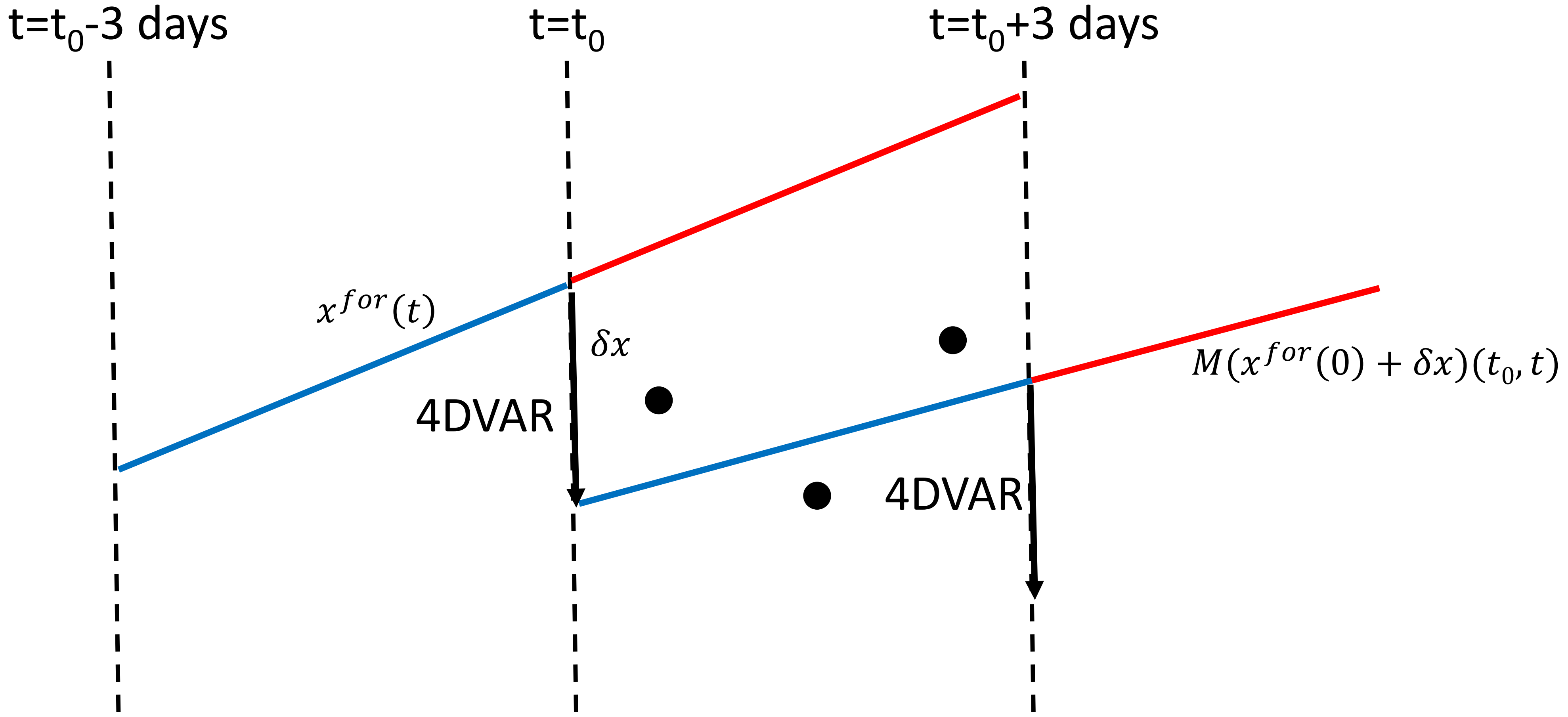
Motivation

NANOOS model: ingria.coas.oregonstate.edu/rtdav/

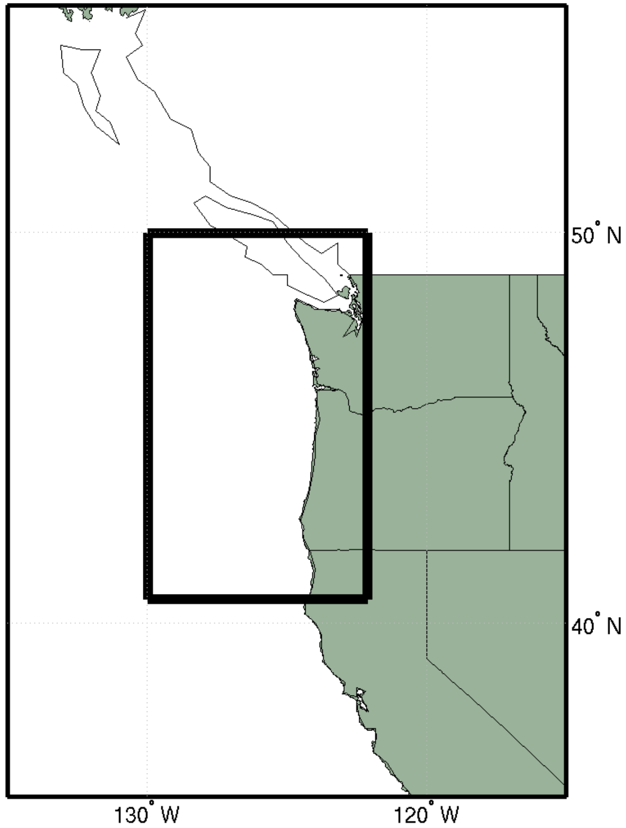
Developed by: L. Erofeeva, A. Kurapov, I. Pasmans and P. Yu



Current forecasting system



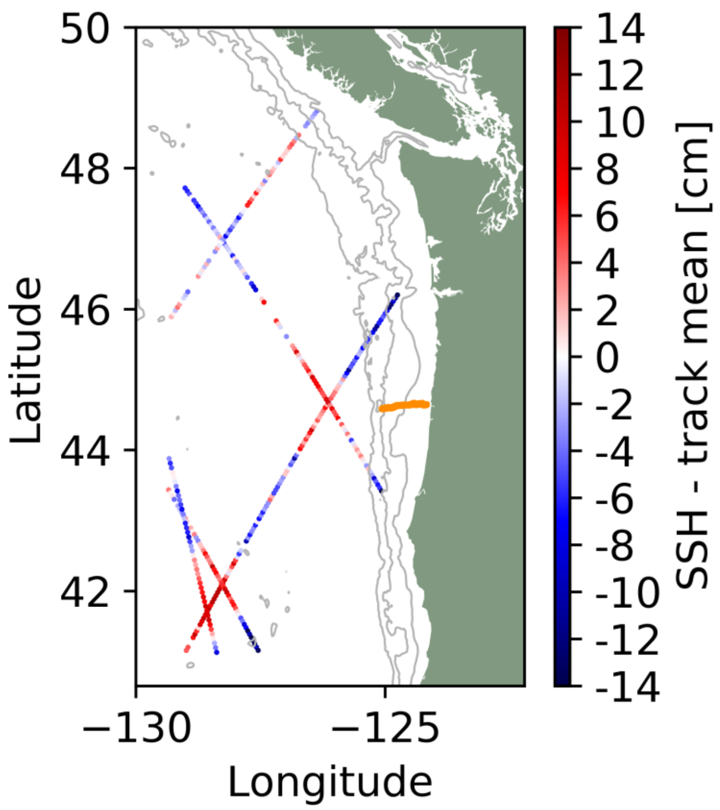
Nonlinear model



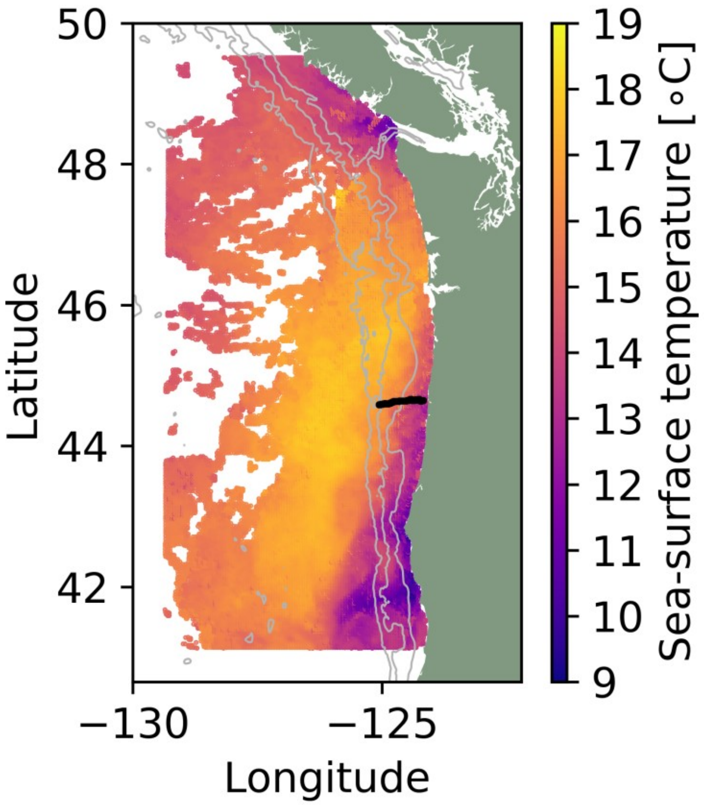
- Kim et al., 2014
- ROMS model
- 3D nonlinear hydrostatic Boussinesq model
- 2km resolution Arakaw-C grid
- 40 terrain following layers
- North American Model (NAM) wind forcing
- HYCOM boundary conditions
- TOPEX tides ad boundaries (Egbert et al., 1994; Egbert and Erofeeva, 2002)

Assimilated observations

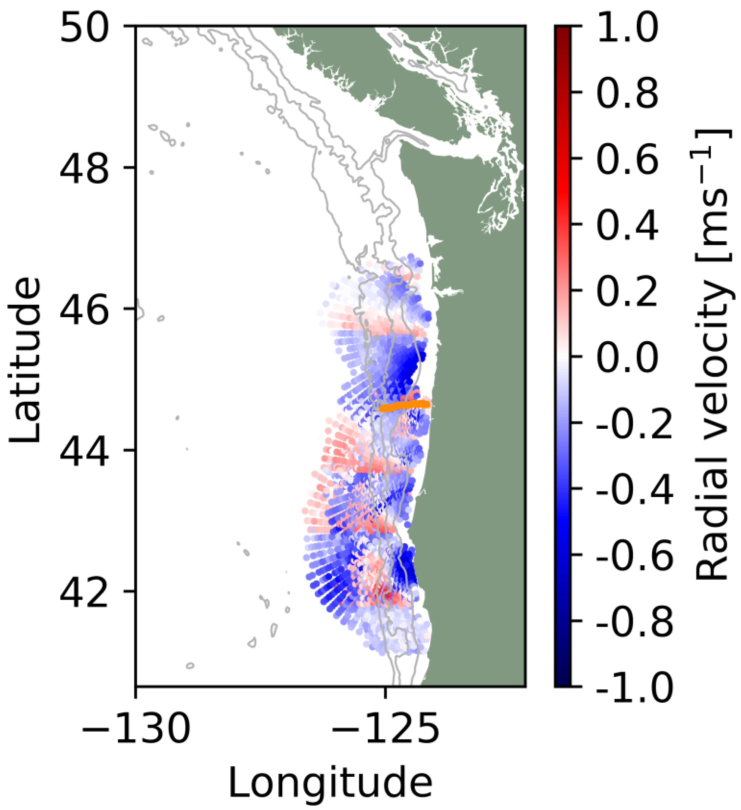
Satellite altimetry (Jason, Cryosat, Envisat)



GOES satellite sea-surface temperature



Radial high-frequency radar sea-surface currents (P. Kosro)

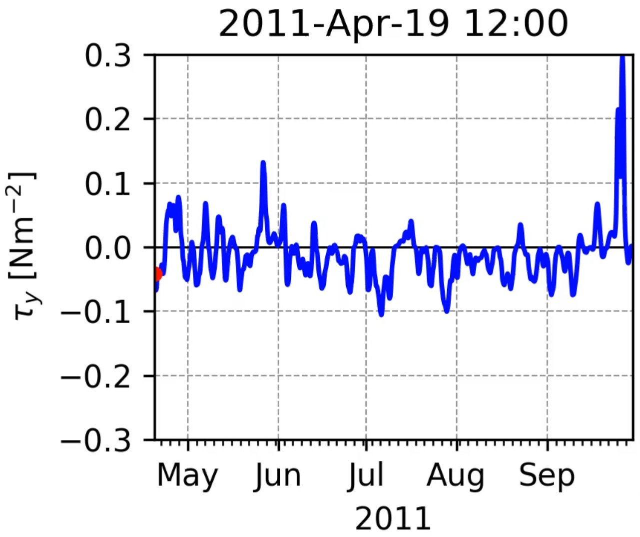


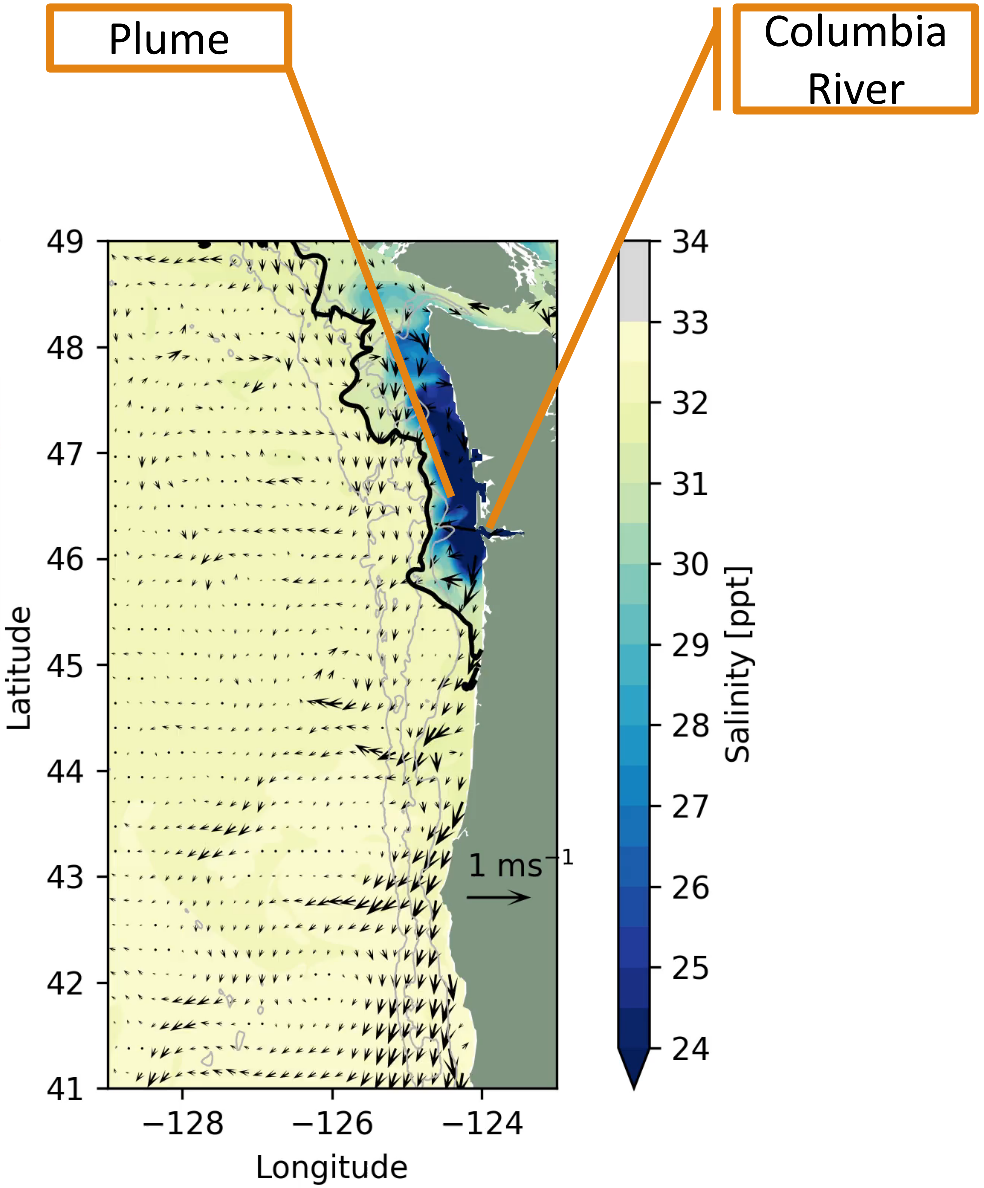
Background error covariance **B**

- 4DVAR performed by the in-house developed AVRORA code
- Balance operator covariance (Weaver et al., 2005)
  - Simple, fixed T,S error relation ($\delta S = -\alpha\delta T, \alpha = 0.16\frac{psu}{C^{\circ}}$) from T,S-diagram
  - Linear equation of state
  - Thermal wind balance
  - No correction to depth-integrated transport
- Static in time.

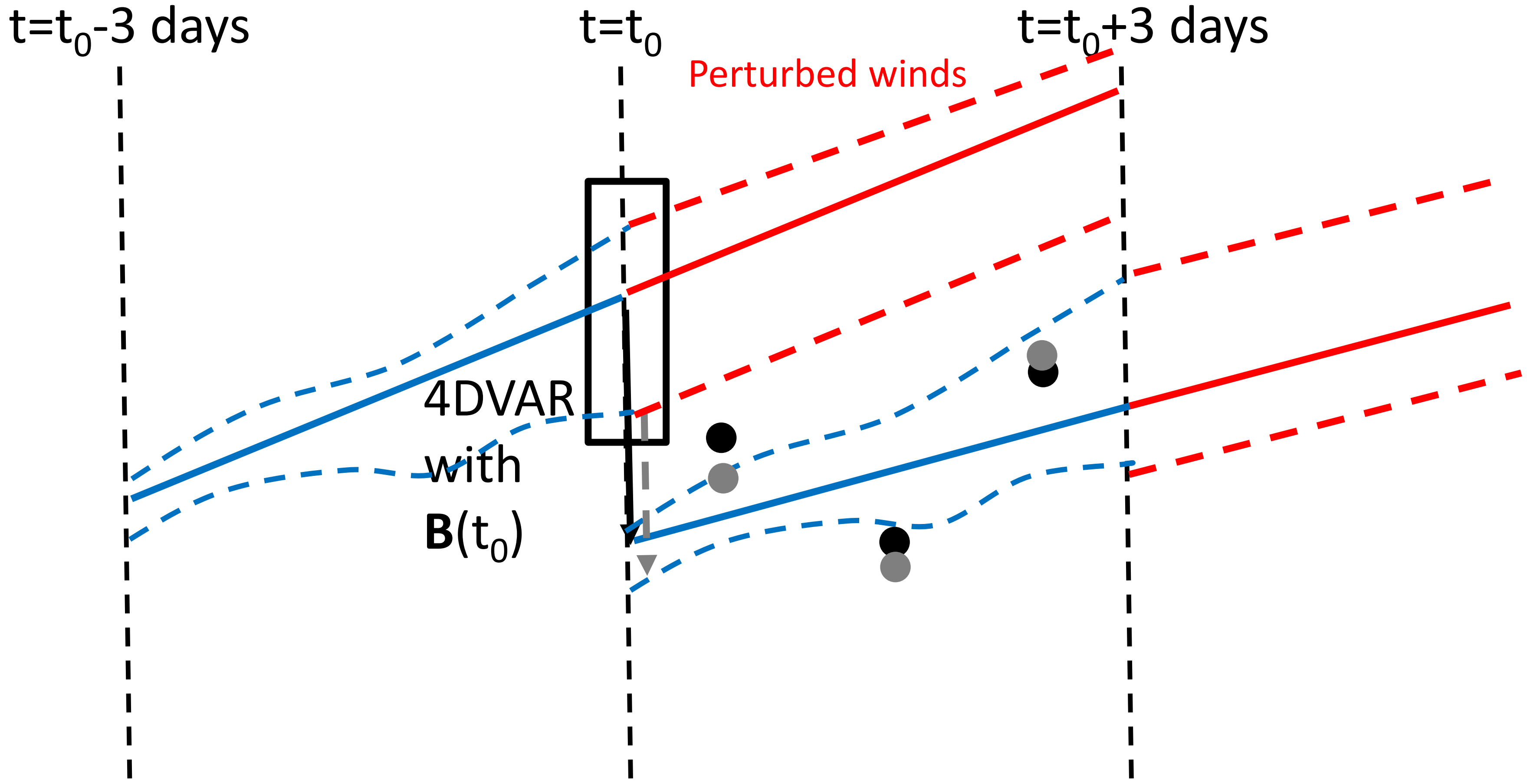
Regional dynamics

- Strongly variable on regional and short time scales
- Southerly winds:
  - River plume flows northward
- Northerly winds:
  - River plume turns south
  - Upwelling deep ocean water ($\rho \geq 1026.5\ kgm^{-3}$)
  - Upwelling moves plume in offshore direction
- Time scale system: 2-10 days (Hickey et al.,1998)





E4DVAR method



- Perturbed observations for ensemble members. (Houtekamer and Mitchell, 1998).
- Monte-Carlo localization (Pasmans and Kurapov, 2017).
- Restricted B-conjugate gradient (Gürol et al., 2014) preconditioning.
- Parallel expansion of the search space in which a iterative solution is sought.
- Lower-rank approximation inverse reused for ensemble members (similar to S-EVIL, Auligné et al., 2016) .

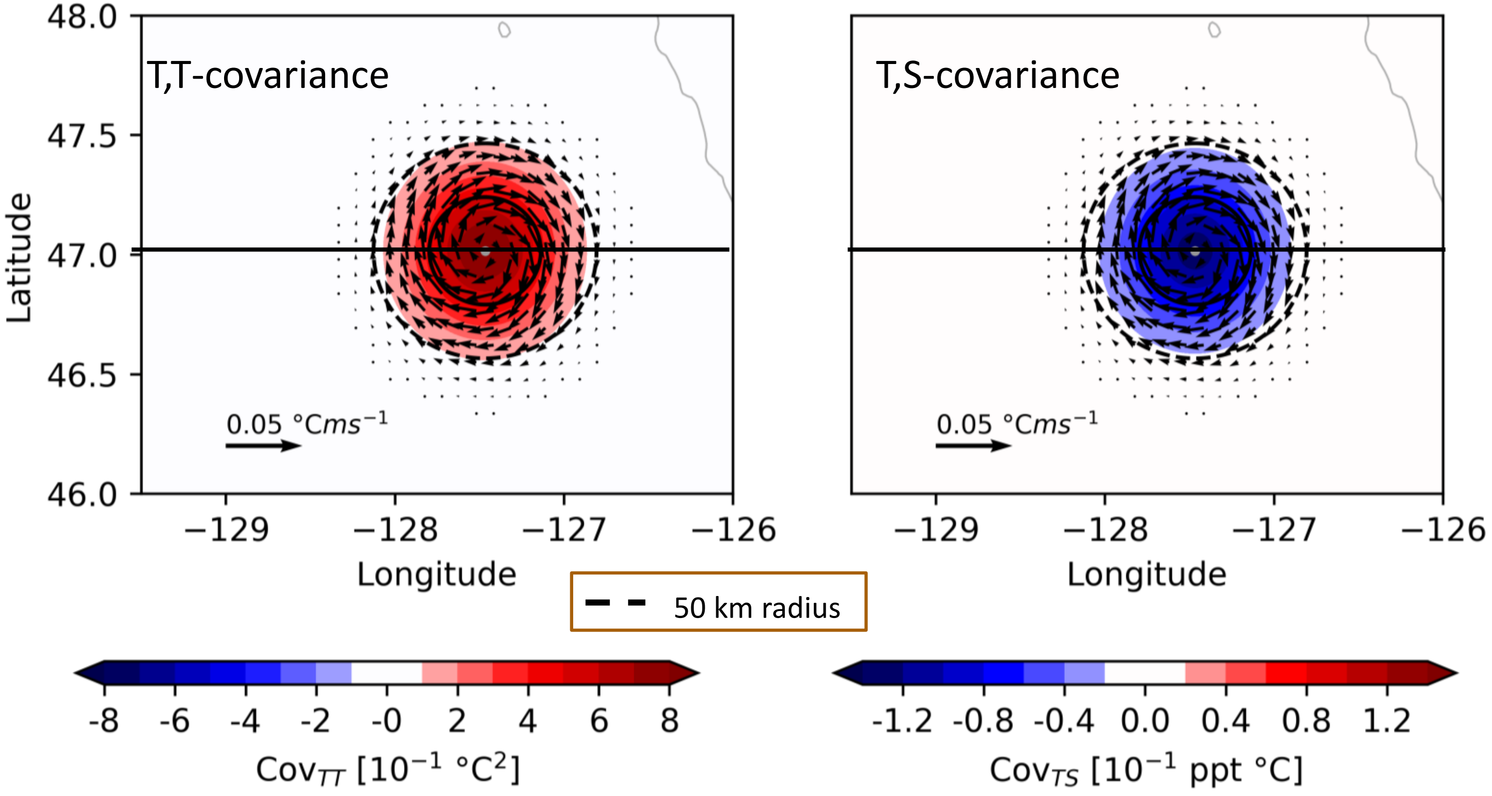
Outline

- Compare covariances from the balance operator **B** with ensemble **B.**
- Compare model result with respect to
  - Assimilated observations
  - Independent T,S-buoy observations
  - Glider T,S-relation
- Present salinity constraining scheme.

- Experiments 19 April 2011-1 October 2011:
  - No data assimilation (*No DA*)
  - **B** constructed from an ensemble (*Ens*)
  - **B** constructed from an ensemble with a scheme controlling salinity corrections (*Ens-con*)
  - **B** constructed using the balance operator covariance with a scheme controlling salinity corrections (*Bal-con*)

Open ocean balance operator covariance

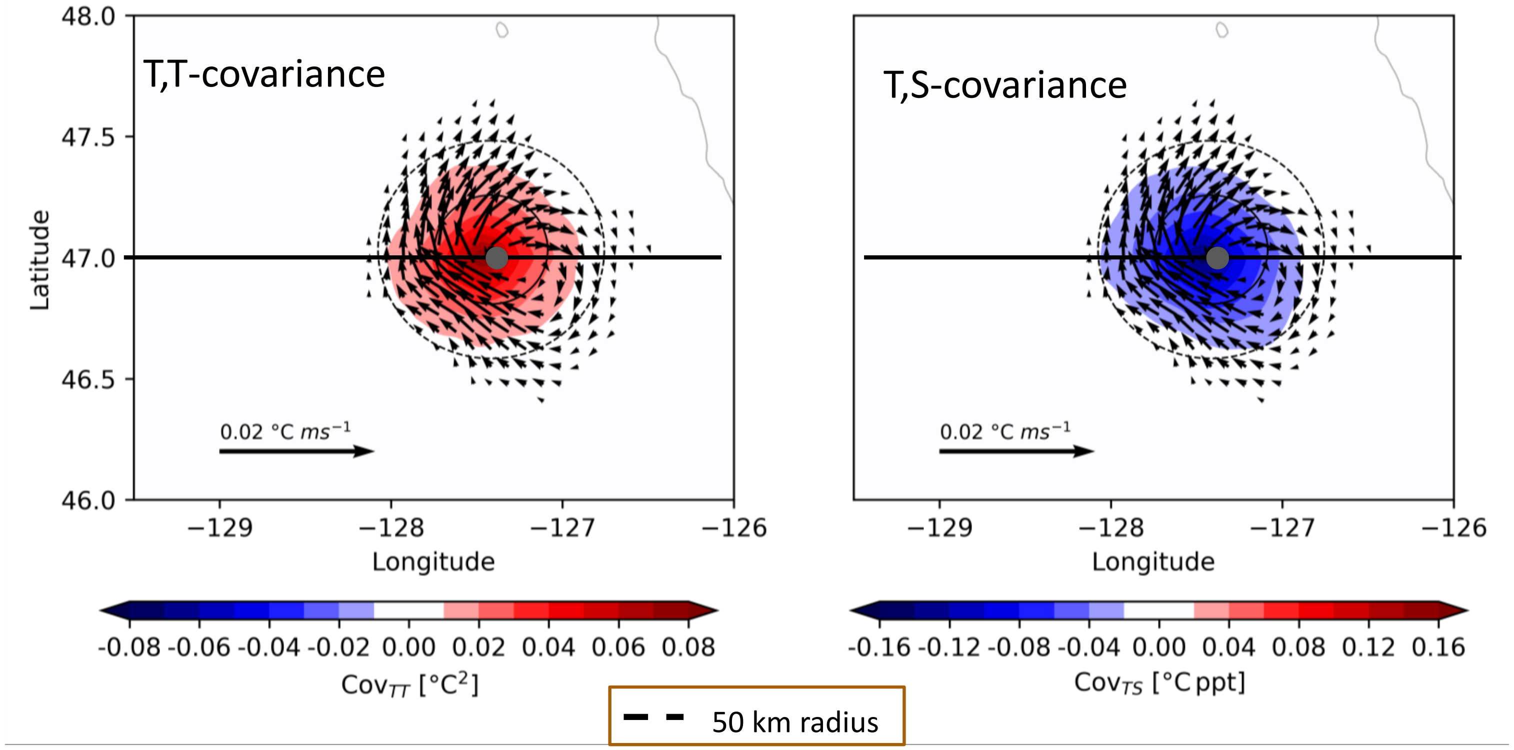
Balance operator SST,· -covariances



Ensemble covariance: open ocean

On average localized ensemble covariance reproduces the balance operator covariance, but with a T-variance a factor 10 smaller.

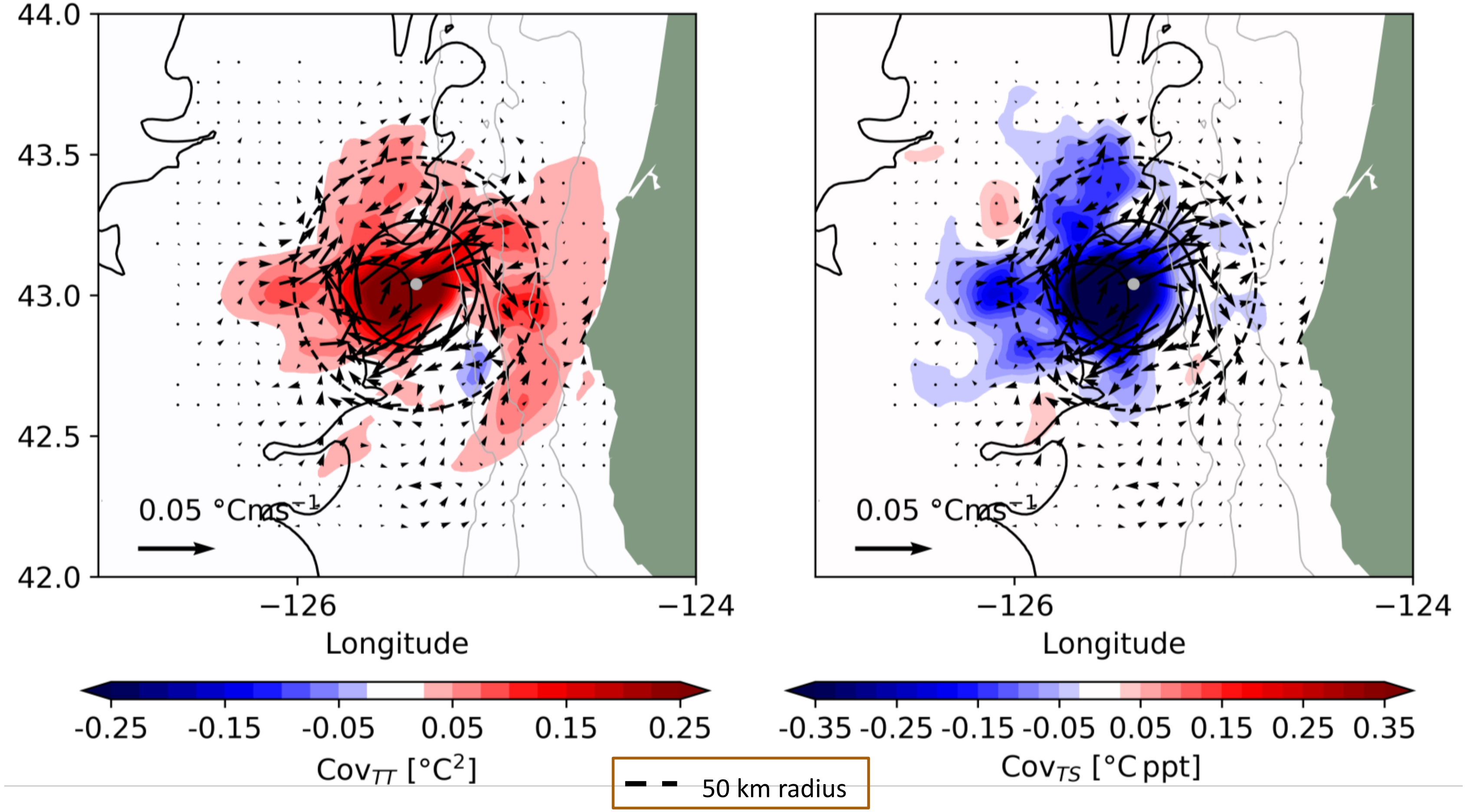
Averaged localized SST,· -covariances



Ensemble covariance: fronts

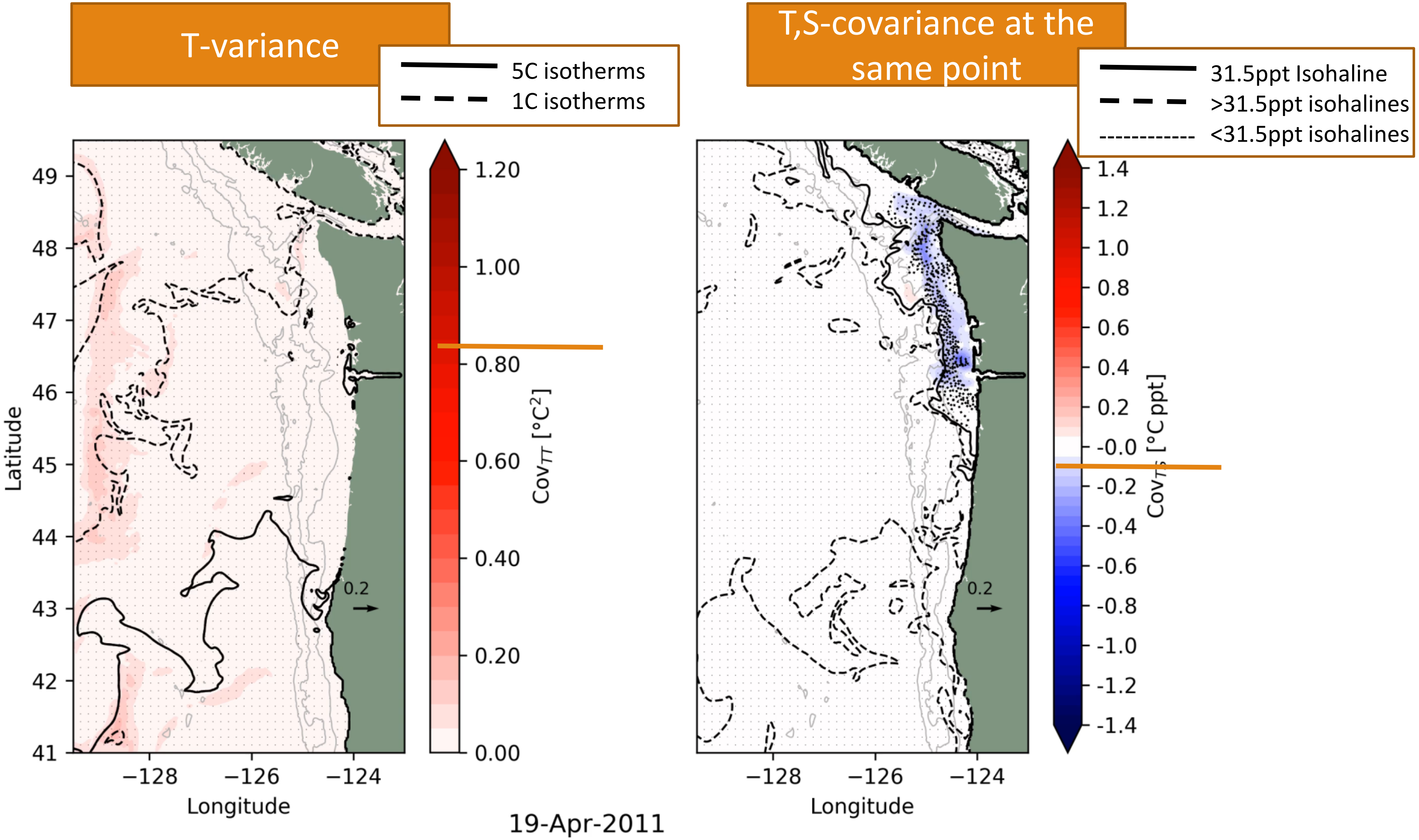
- Temperature correlated with cross-front velocities instead of anti-cyclonic velocities.

Localized SST,· -ensemble covariance 9 July 2011



Ensemble surface (co)variance

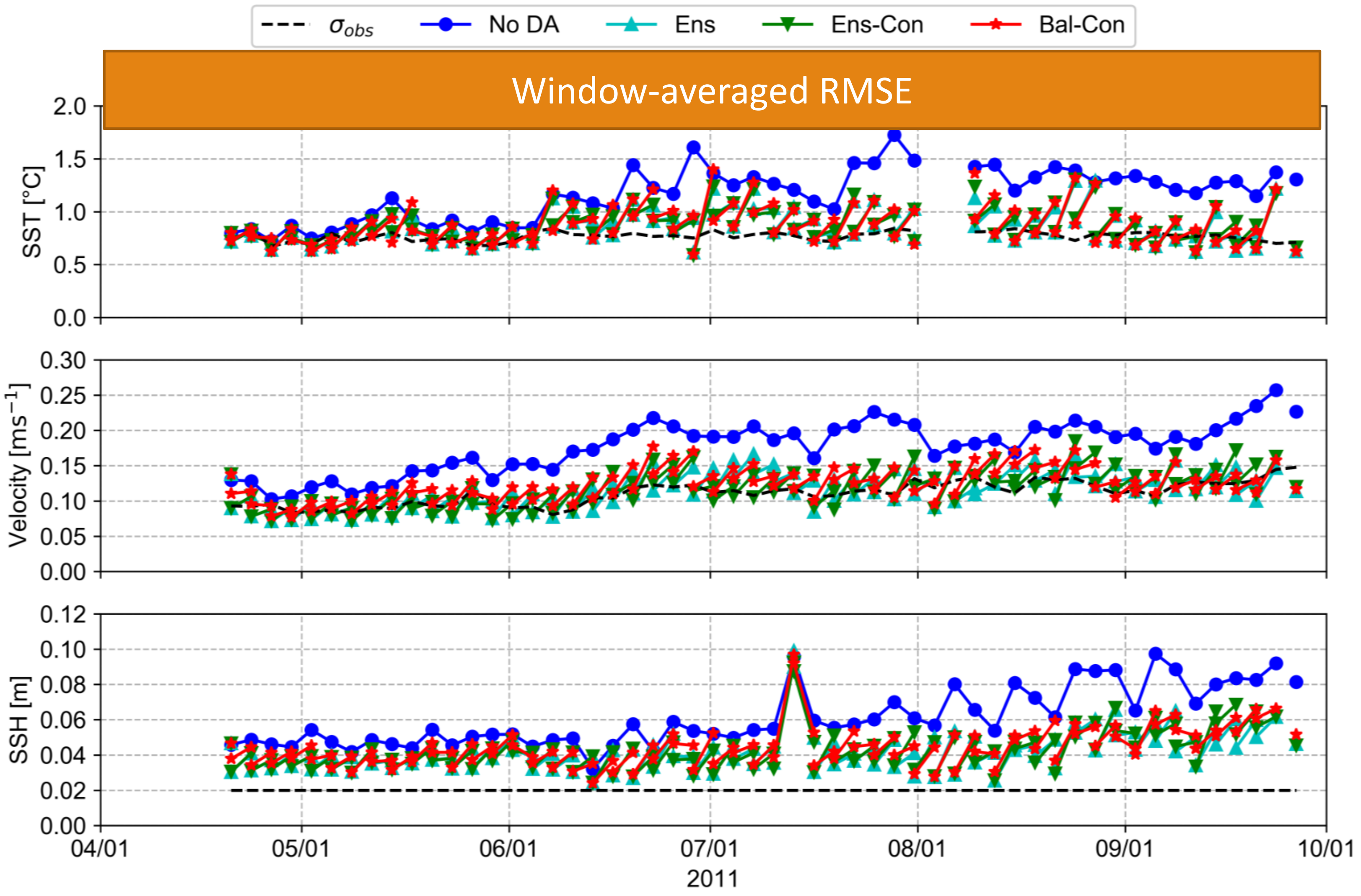
- General magnitude T-variance and T,S-covariance smaller than balance operator equivalents (0.81°C^2, -0.13 ppt $^{\circ}$C)
- Large magnitudes near fronts.
- Large magnitudes *T* and *S* at different locations.



Analysis-forecast RMSE per window

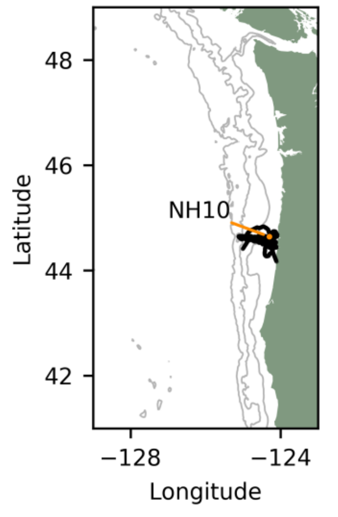
- DA reduces errors in analyses and forecasts
- E4DVAR slightly outperforms Balance Operator covariance.

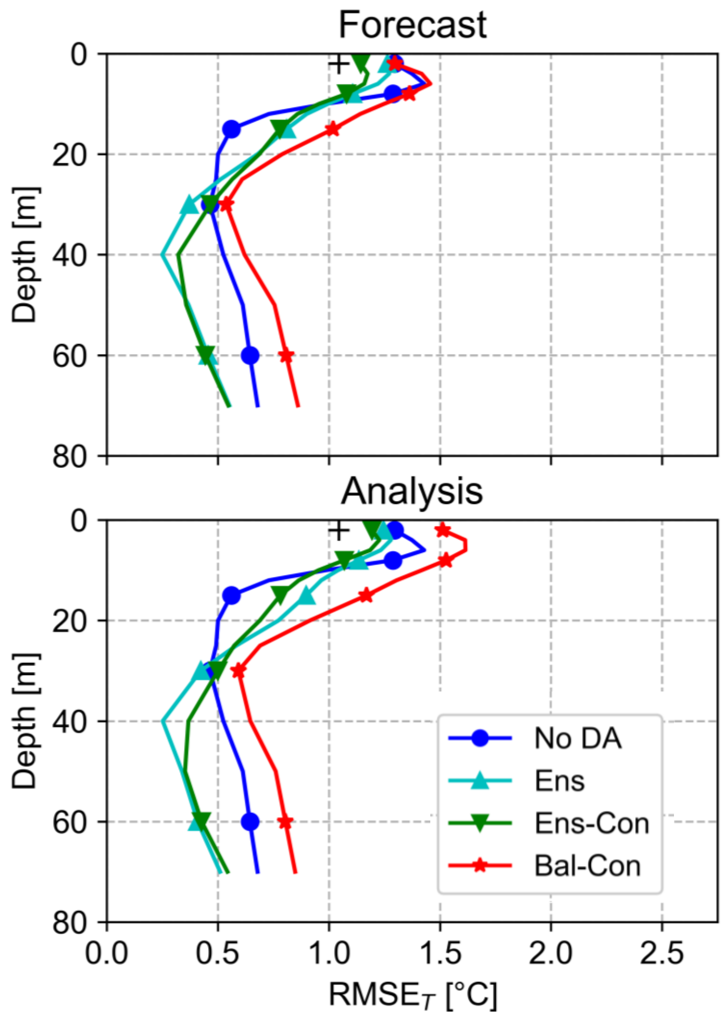
Experiment	SST [C]	u [m/s]	SSH [m]
σ	0.768	0.112	0.020
No DA	1.189	0.180	0.063
B ens	0.775 0.963	0.104 0.131	0.038 0.049
B ens-con	0.777 0.970	0.104 0.133	0.039 0.049
B bal-con	0.763 1.001	0.114 0.137	0.042 0.050



NH10 comparison

- E4DVAR as accurate as satellite SST (+) near surface.
- E4DVAR more accurate below the surface layer.
- Balance Operator performance deteriorates if no satellite SST observations near NH10 are present.



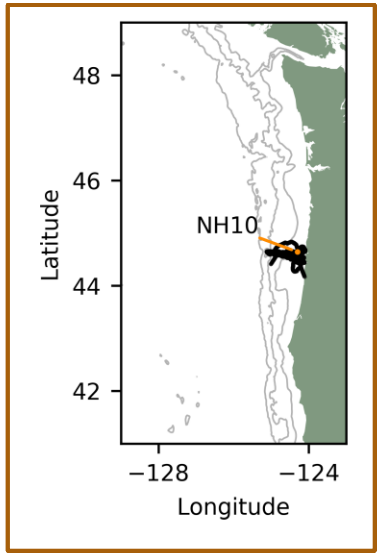


Average RMSE 4/19-10/1

Image source: http://www.ndbc.noaa.gov/station_page.php?station=46094

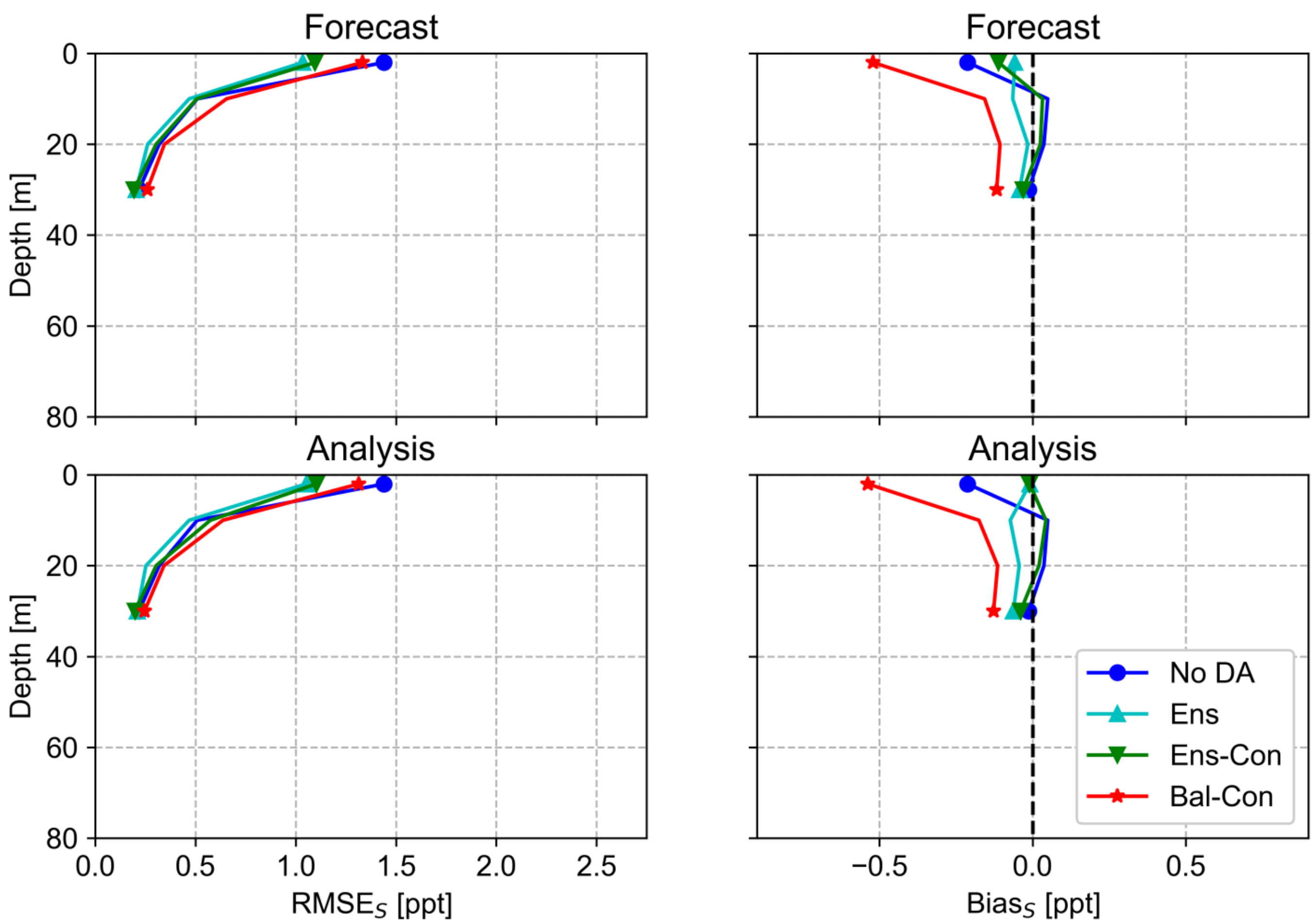
NH10 comparison

- E4DVAR produces more accurate results for salinity near the surface.



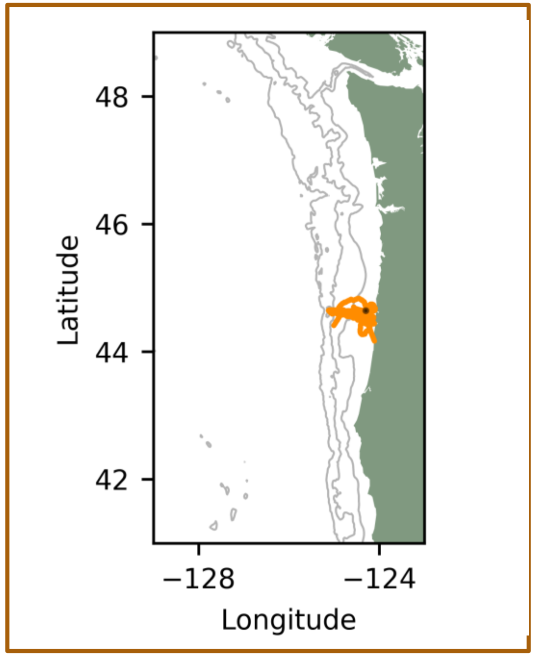
Average RMSE 4/19-10/1

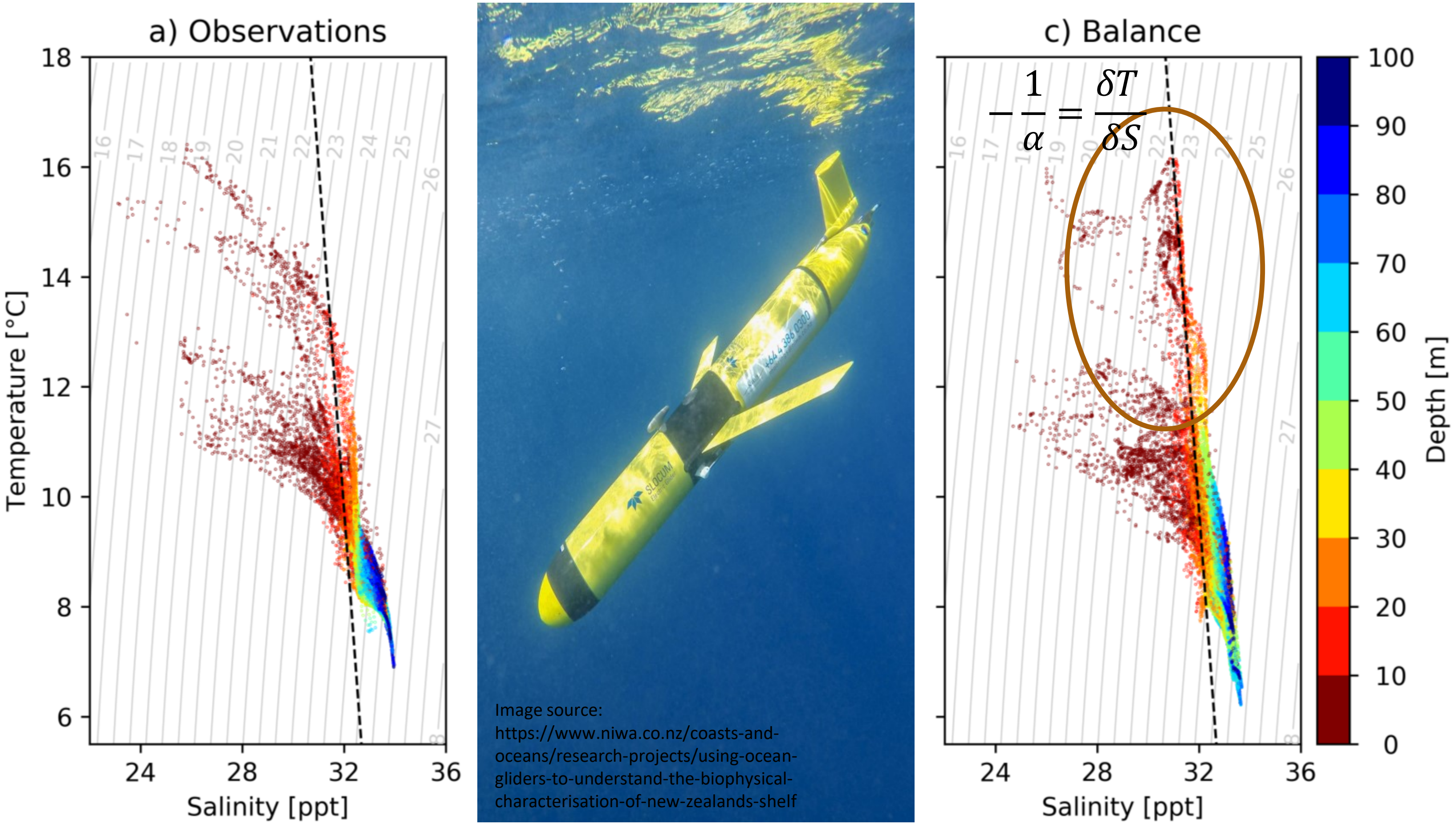
Average bias 4/19-10/1



T,S-relation

- Deformation T,S-relation using Balance Operator
- Using E4DVAR removes deformation

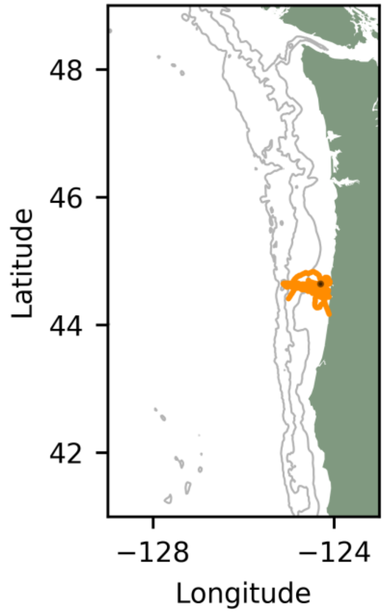


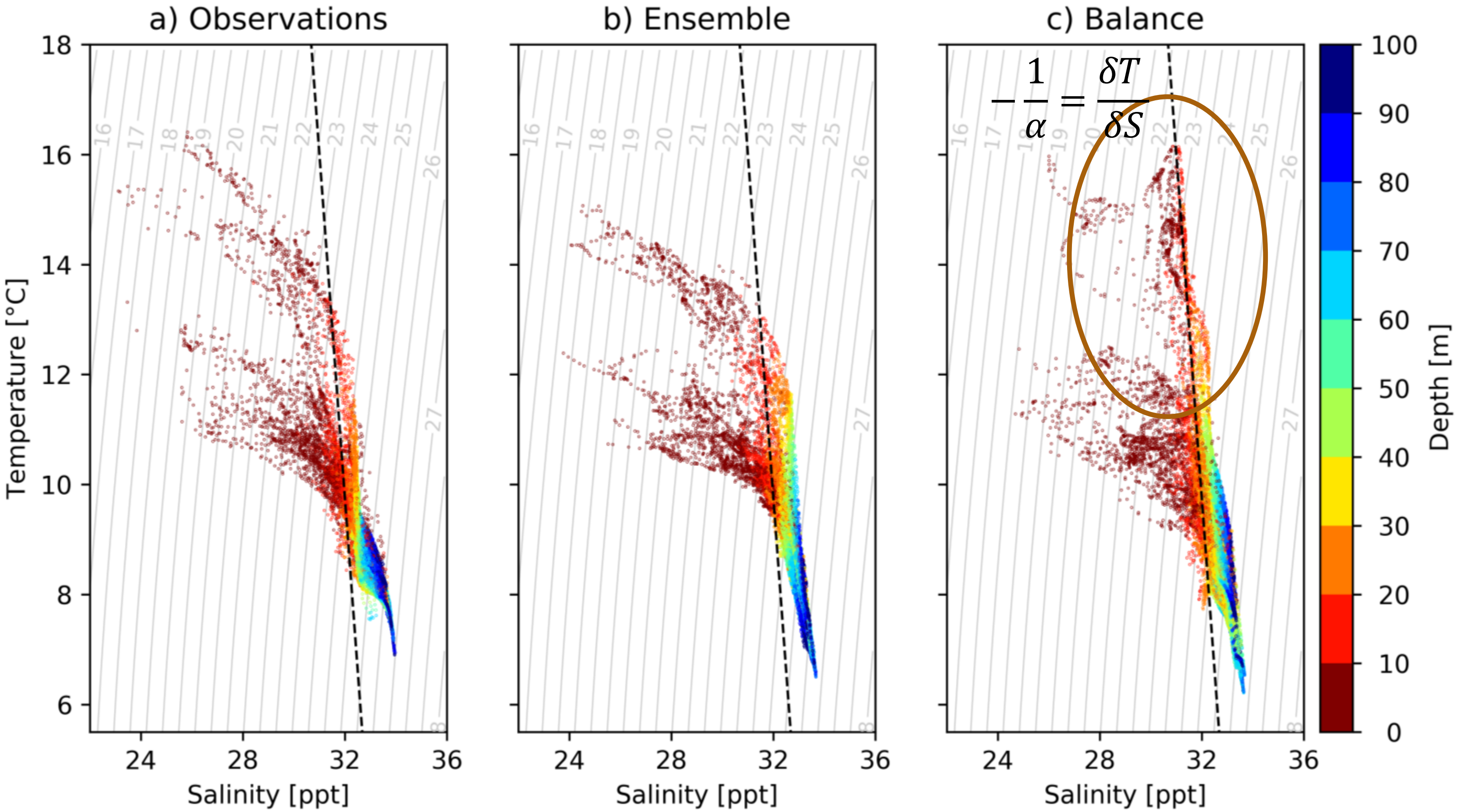


Forecasts 19 April 2011-30 June 2011

T,S-relation

- Deformation T,S-relation using Balance Operator
- Using E4DVAR removes deformation

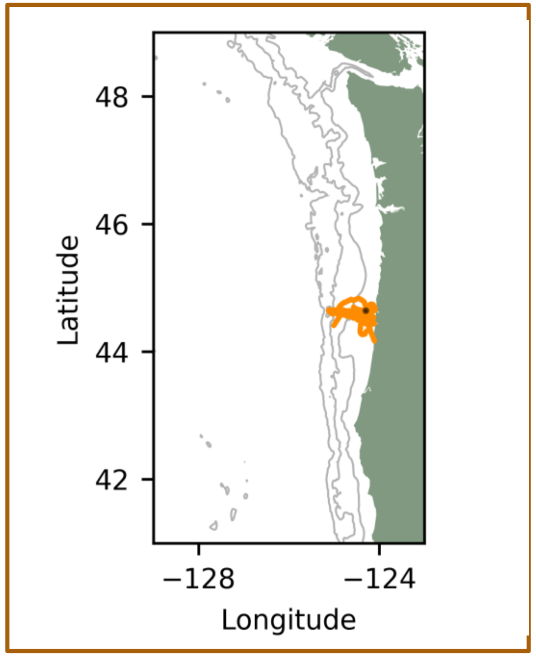


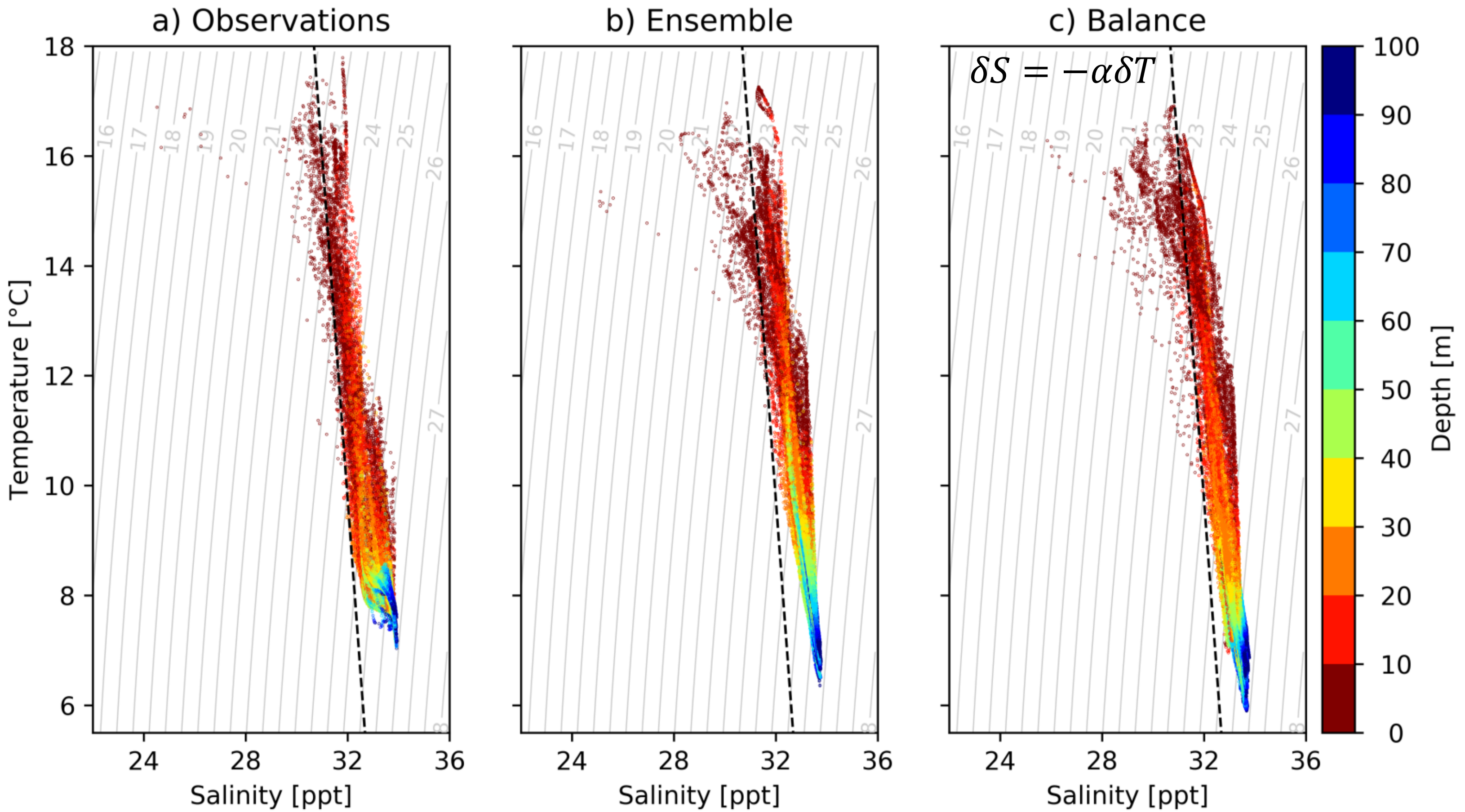


Forecasts 19 April 2011-30 June 2011

T,S-relation

- E4DVAR correctly captures T,S-relation when it reverts to -0.16 ppt/°C

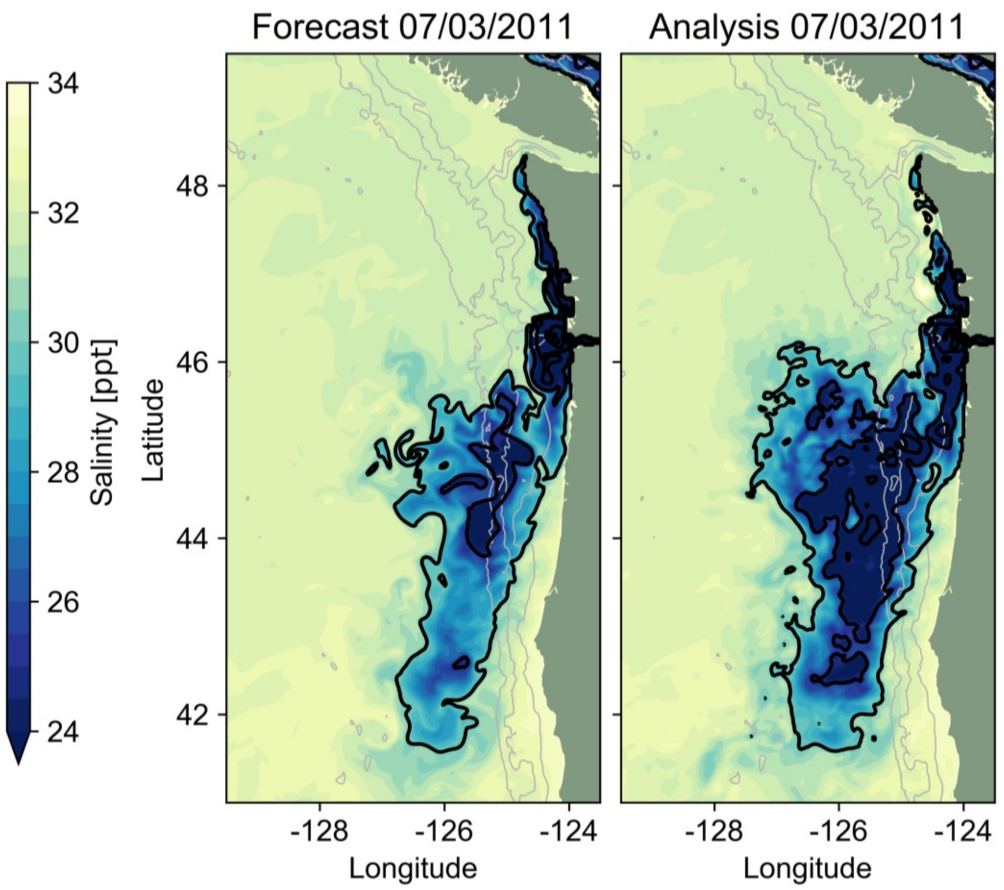




Forecasts 1 July 2011 – 1 October 2011

DA induces large corrections plume size

No constraint on salinity



- Assimilation with ensemble **B** can instantly increase/decrease the size of the plume → violation conservation salinity.

Salinity constraining scheme

- Divide domain up into a hierarchy of boxes of different sizes.
- Add penalty to the cost-function for DA induced changes in average salinity of each box.
- Large-scale changes in surface salinity cause the total salinity penalty to increase exponentially.

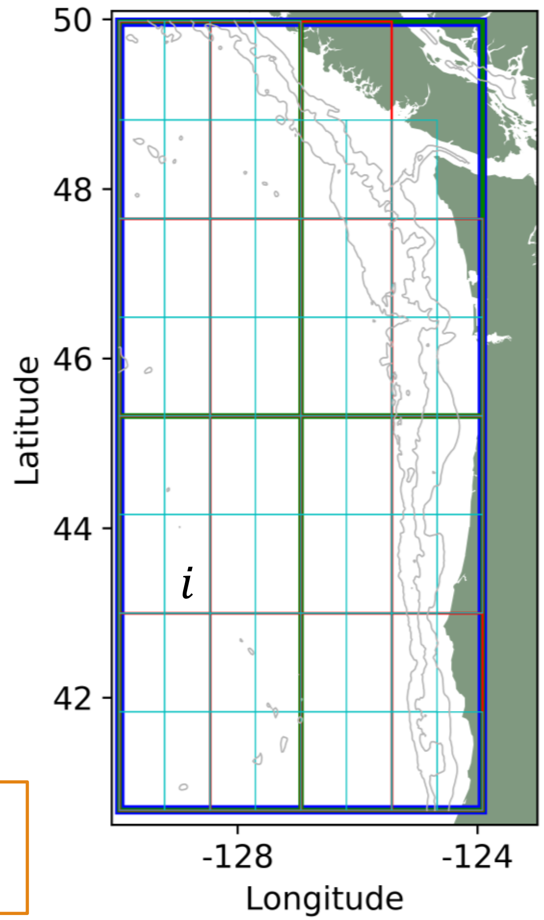
Change average salinity due to DA

$$J' = J + \sum_i \frac{\left(\langle S\rangle_{ana,i} - \langle S\rangle_{for,i}\right)^2}{\sigma_i^2}$$

$$< S >_i = \frac{1}{A_i} \int_{A_i} S \,\mathrm{dA}$$

Weighting based on variability in *No DA*

Salinity boxes



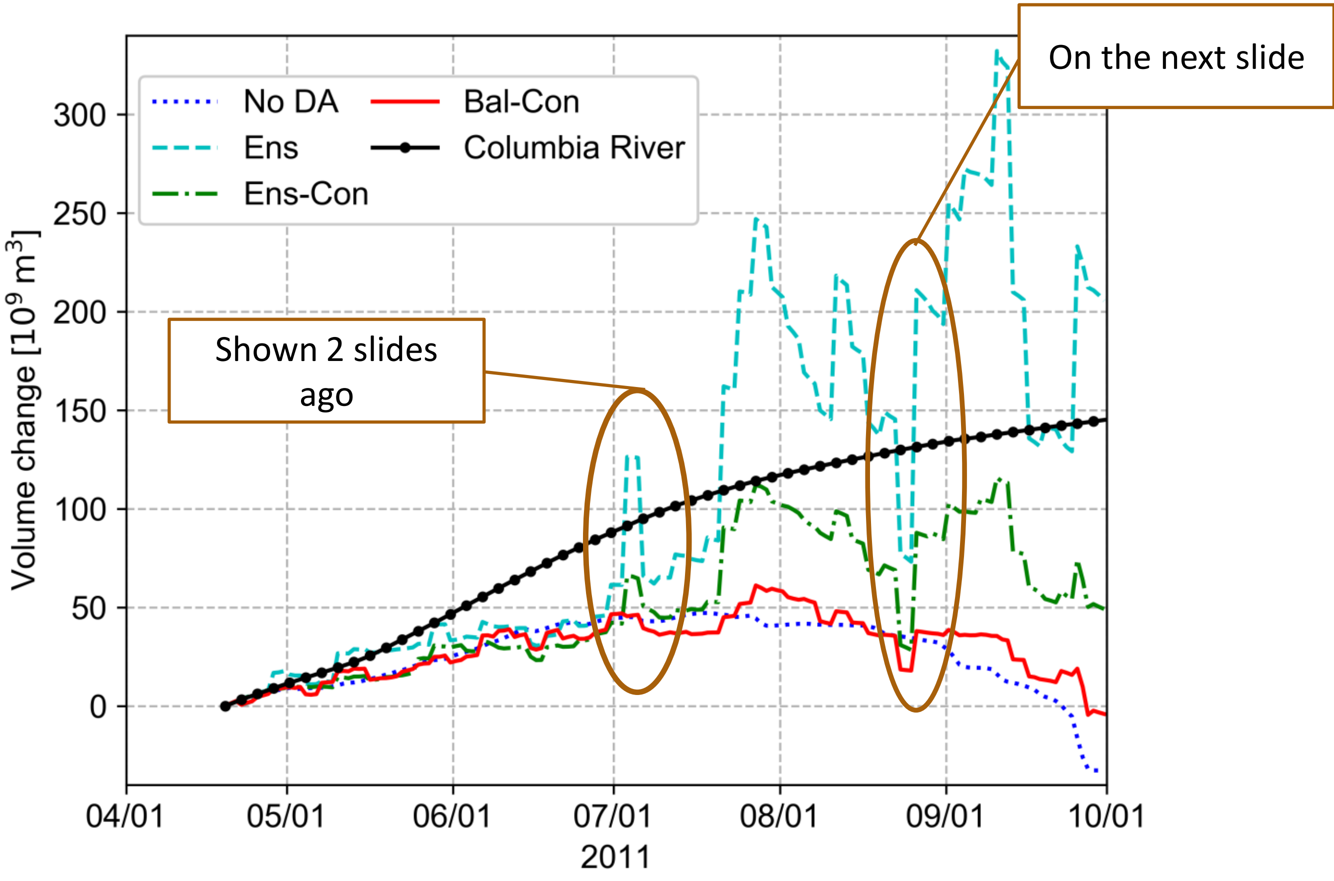
Constraining affects DA changes plume

- Constraining salinity drastically reduces changes in plume water volume by data assimilation.
- Constraining does not completely eliminate the changes to plume water volume by DA.

Find plume water volume per grid cell by solving

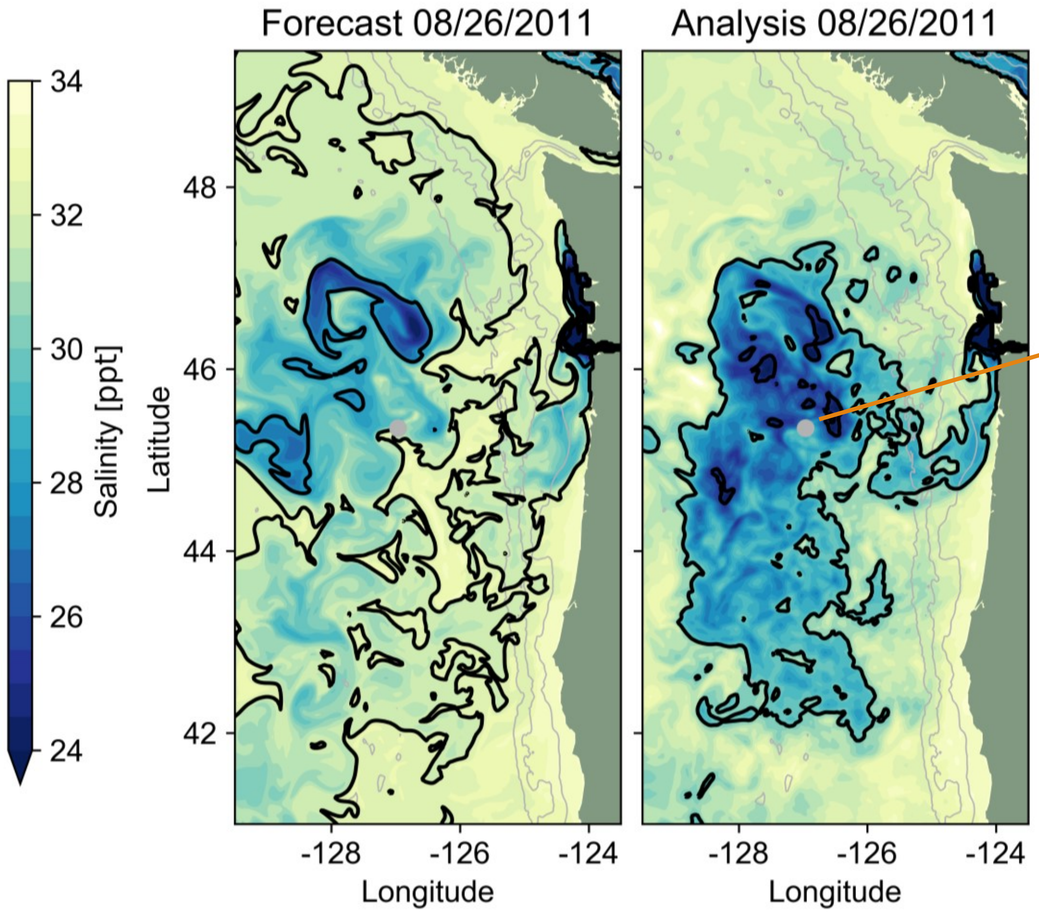
$$S_{grid\ cell}V_{grid\ cell}$$
$$= S_{fresh}V_{fresh} + S_{ocean}(V_{grid\ cell} - V_{fresh})$$
$$S_{fresh} = 0.3\ ppt, S_{ocean} = 32.2\ ppt$$

Plume water volume south of the Columbia River



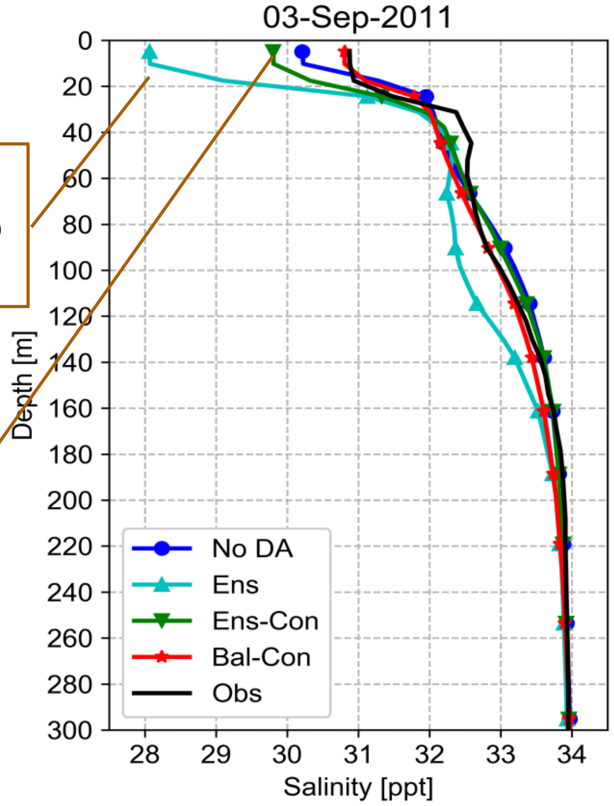
DA corrections are not physical.

No constraint on salinity



- Comparison with Argo float shows that the large DA corrections to salinity reduce surface salinity too much.

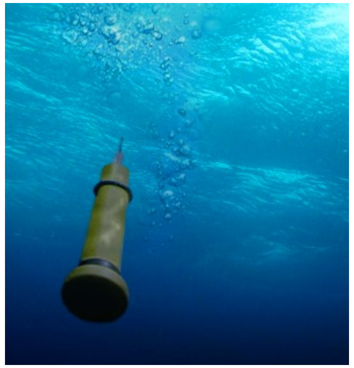
ARGO salinity profile 3 September



Ensemble covariance→too fresh

Constraining improves results

Image source: https://samcharlesjones.files.wordpress.com/2015/07/argo_final2-copy.jpg



Conclusions

- In the presence of a river plume the currently used Balance Operator covariance is not a good approximation for the background error covariance.
- Use of an ensemble-based background error covariance has some benefits over the use of a Balance Operator based background error covariance:
  - Better representation of the T,S-relation along the Newport line.
  - Produces forecasts with lower RMSEs for NH10 and for satellite SST, SSH and HFR surface velocities.
- As a result of the large T,S-covariances in the ensemble covariance, data assimilation corrections to SST can generate unphysical changes in the size and salinity of the plume.
  - Implementing tracer conservation laws as (weak) constraint necessary in future studies.

Questions?

Acknowledgement:
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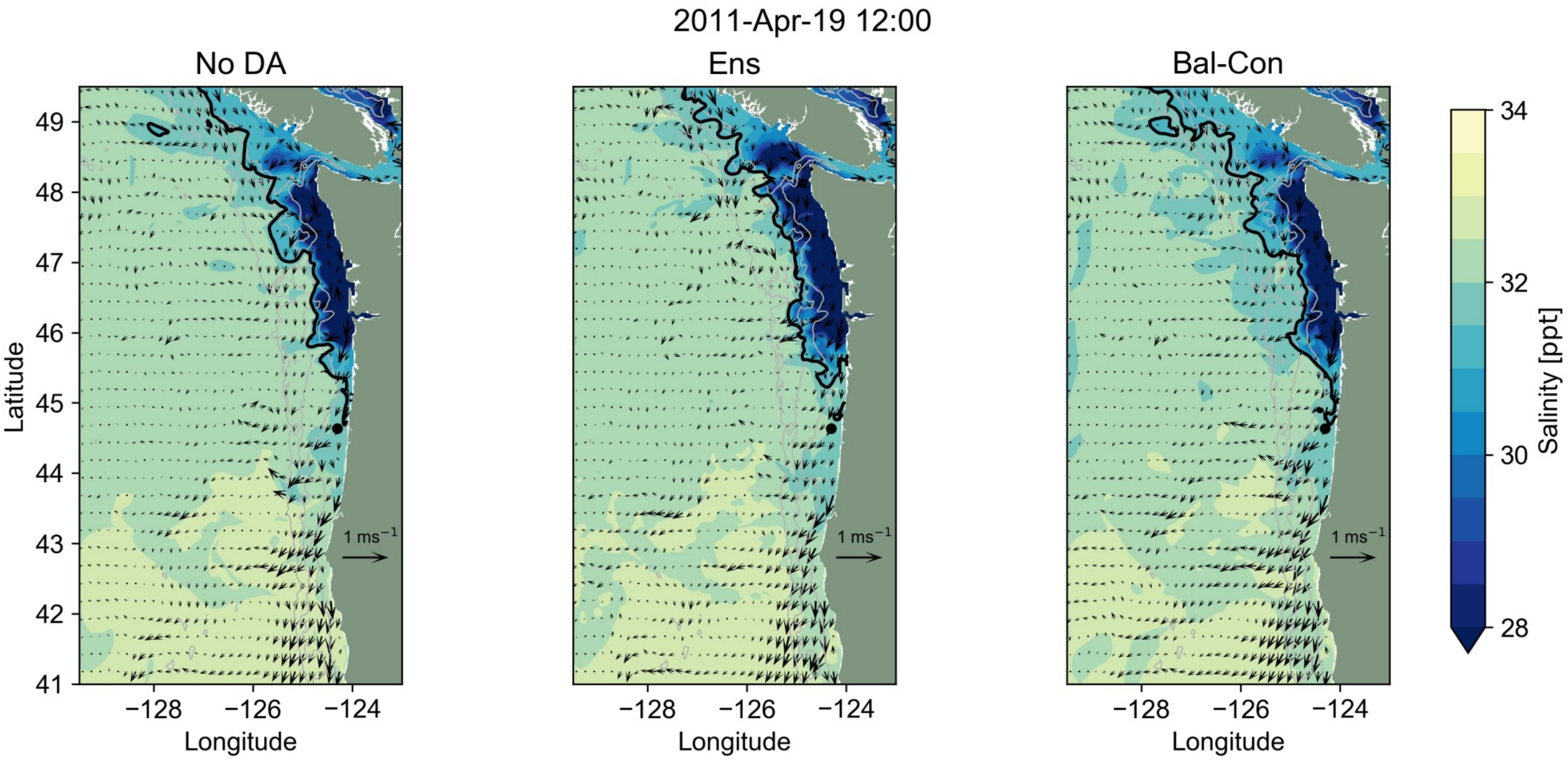
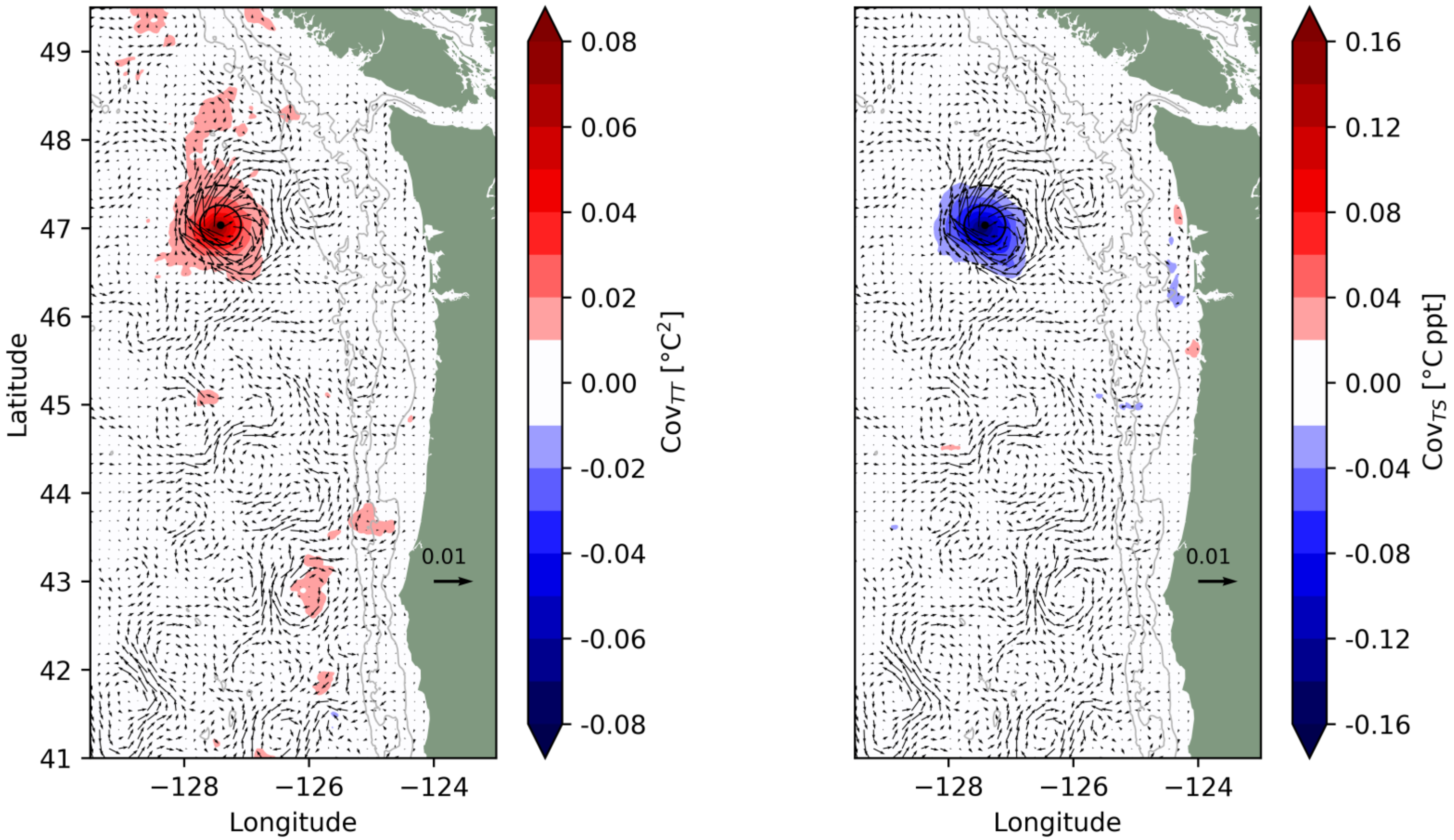
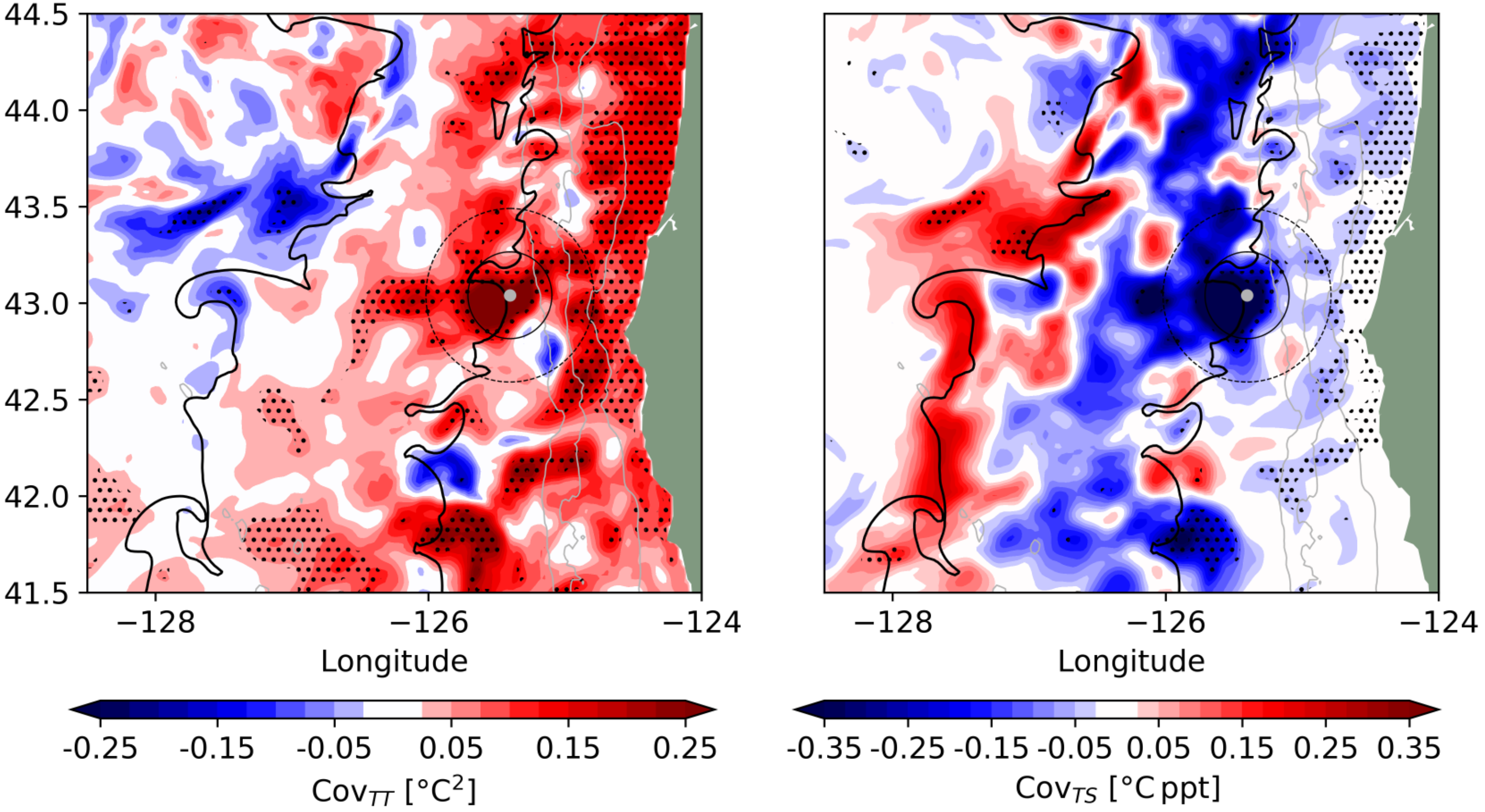
Sea-surface salinity

When using E4DVAR assimilation severely impacts the extend and salinity of the plume.

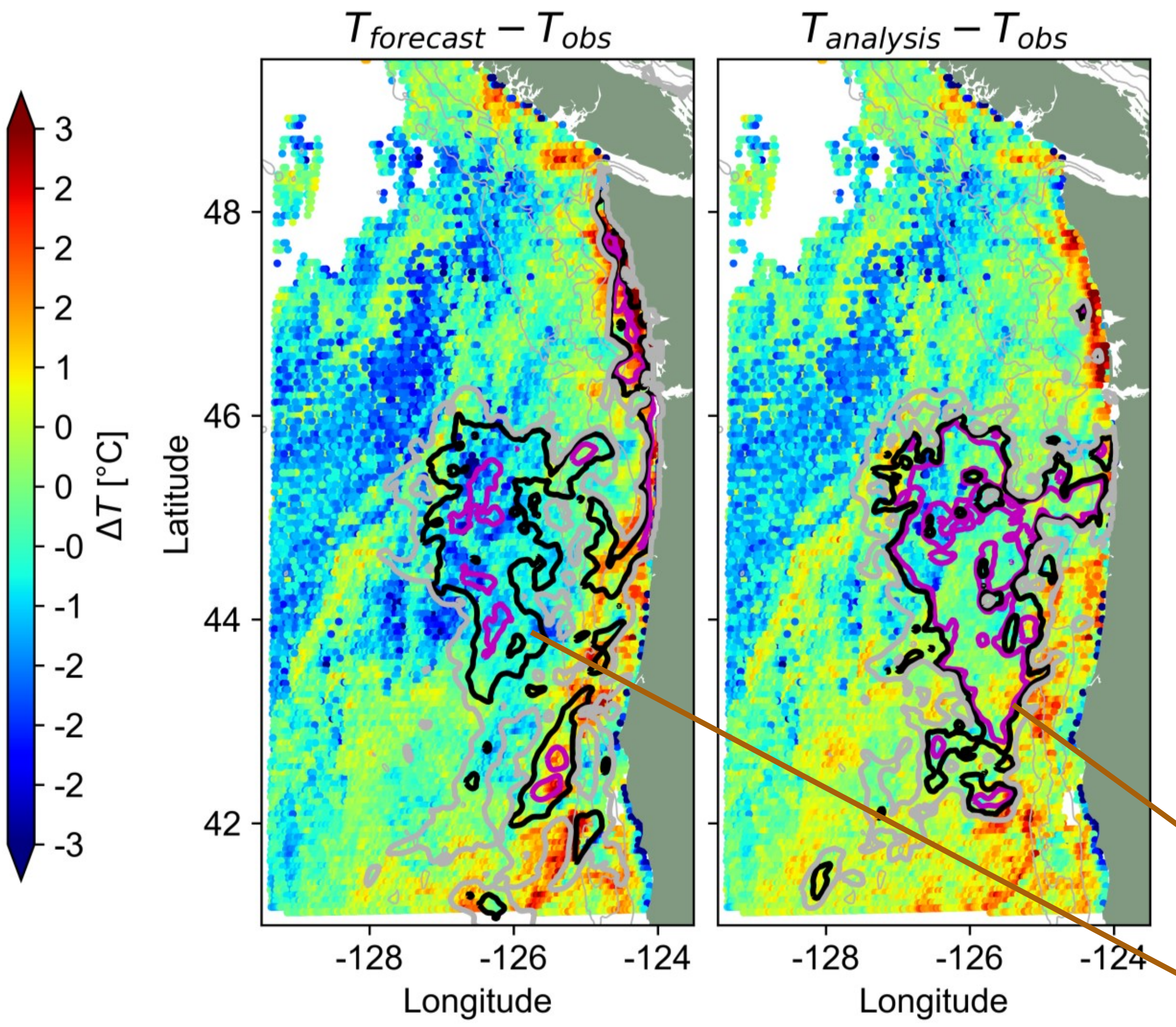
Sea-surface salinity from analyses




49
48
47
46
45
44
43
42
41
Latitude
−128
−126
−124
Longitude
0.01
0.08
0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
-0.08
Cov_{TT} [°C^2]
0.16
0.12
0.08
0.04
0.00
-0.04
-0.08
-0.12
-0.16
Cov_{TS} [°C ppt]


44.5
44.0
43.5
43.0
42.5
42.0
41.5
−128
−126
−124
Longitude
-0.25 -0.15 -0.05 0.05 0.15 0.25
Cov_{TT} [°C^2]
−128
−126
−124
Longitude
-0.35 -0.25 -0.15 -0.05 0.05 0.15 0.25 0.35
Cov_{TS} [°C ppt]

Reason plume size corrections



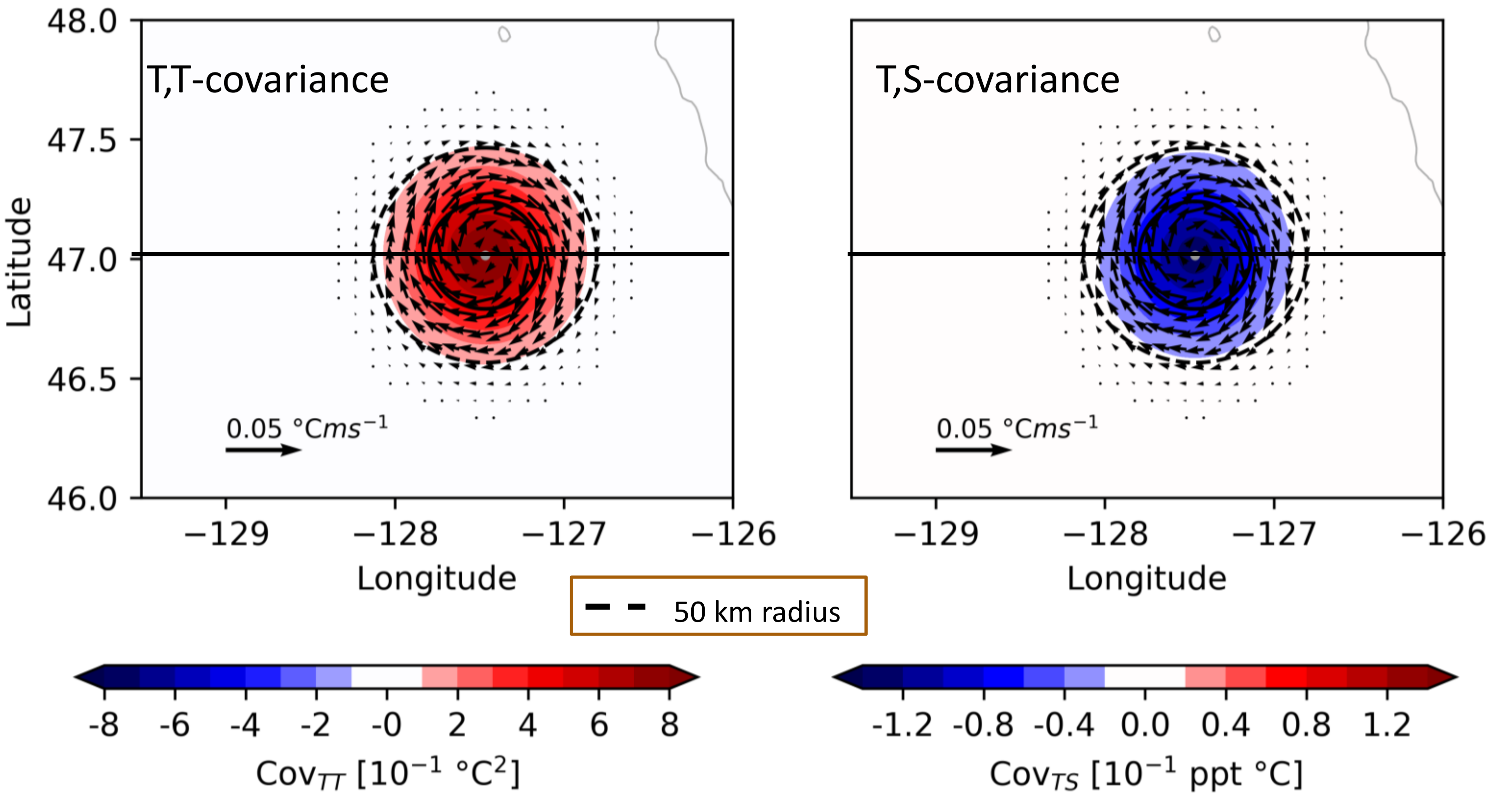
Large salinity corrections are caused by large corrections to SST in combination with the presence of large T,S-covariances.

DA correction to surface salinity (-1,-2,-3 ppt)

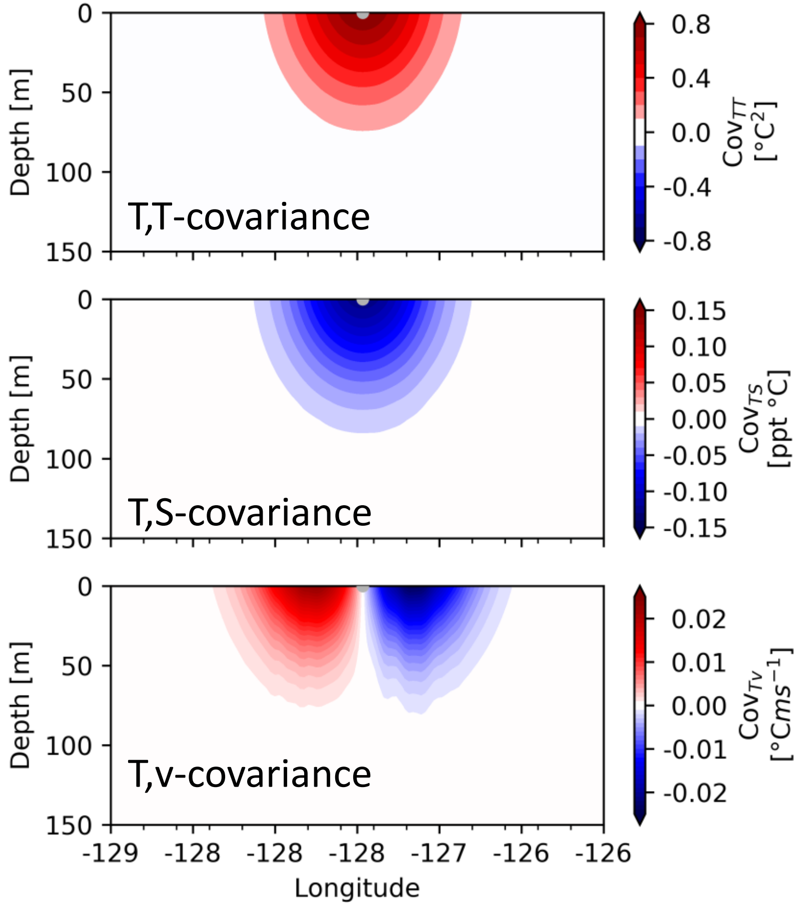
T,S-covariance (1x,2x,4x balance operator covariance)

Open ocean balance operator covariance

Balance operator SST,· -covariances



Balance operator SST,· -covariances along 47°N



Ensemble covariance: open ocean

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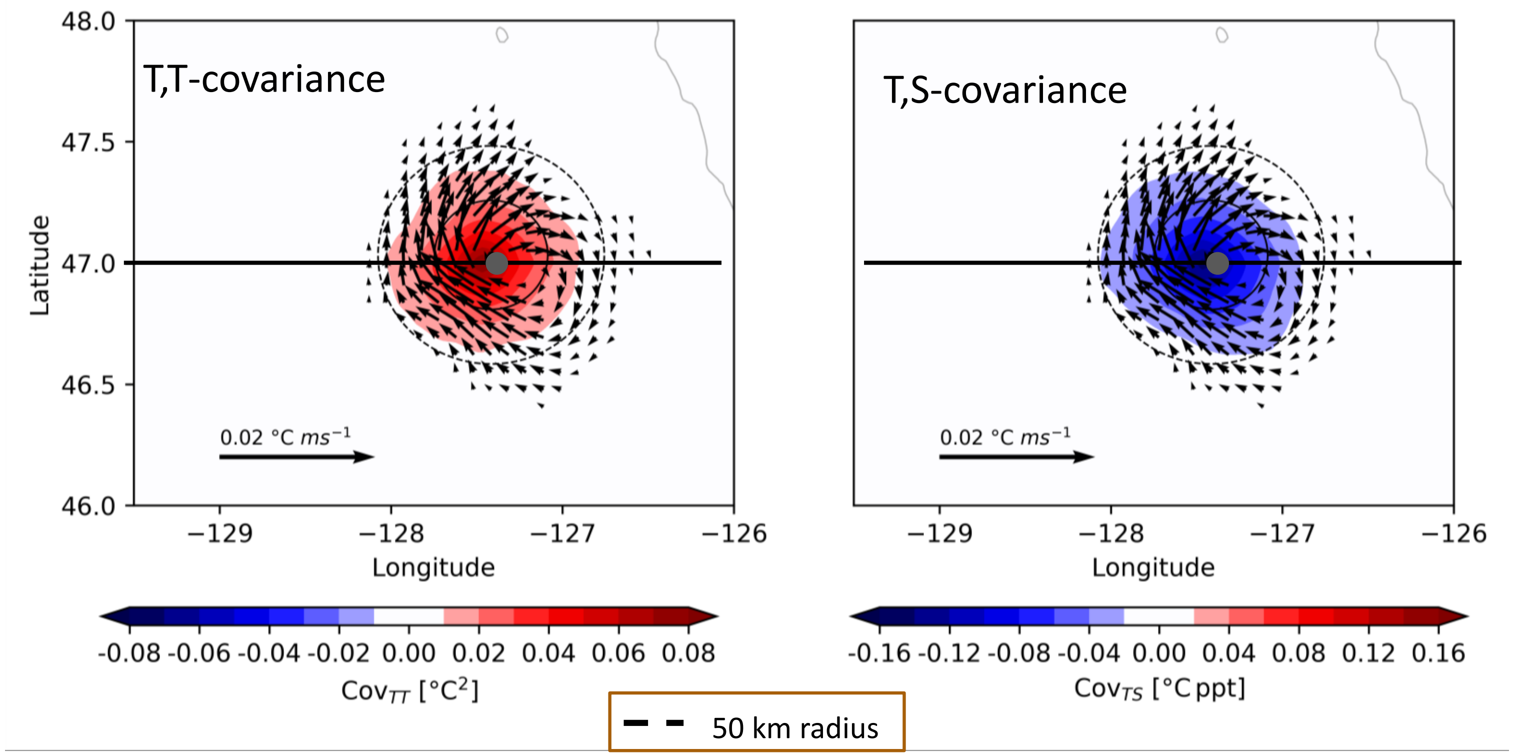
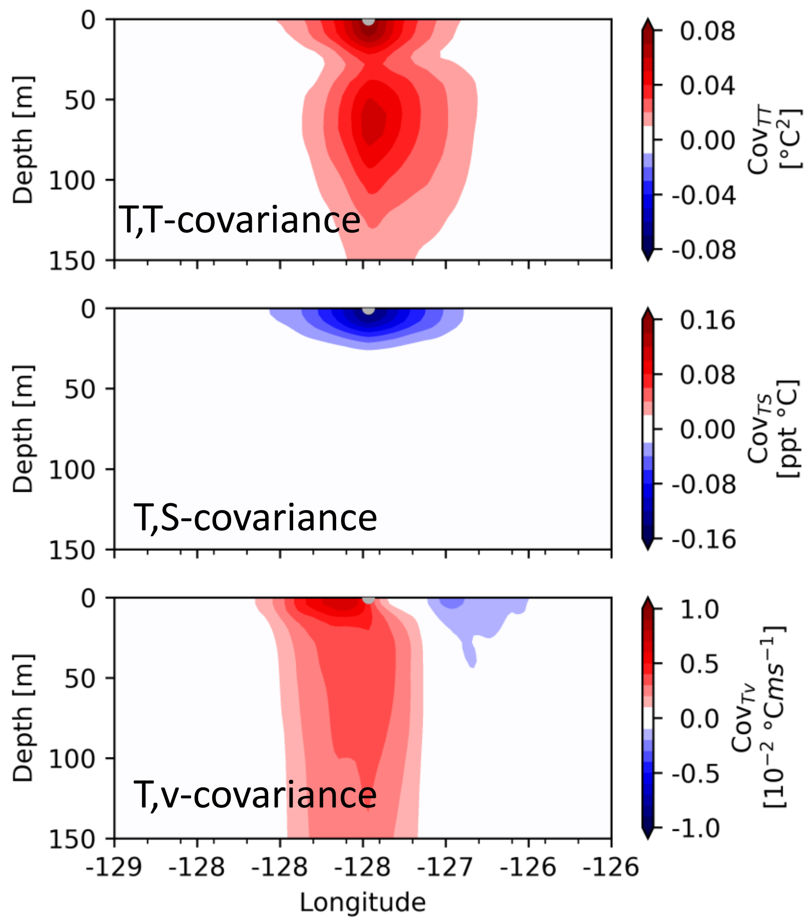
Averaged localized SST,· -covariances



Averaged SST,· -covariances along 47°N



Strong 4DVAR

Model error at the beginning of $\vec{x}_{for}$

Observations

Innovation vector: $\vec{d} = \vec{o} - HM(\vec{x}_{for})$

Assumption that $P(\overrightarrow{\delta x})$, $P(\vec{o} \mid \overrightarrow{\delta x})$ are Gaussian

$P(-\overrightarrow{\delta x}|\vec{o})$ ~ exp(- J($\overrightarrow{\delta x}$))

$$J(\delta x) = \frac{1}{2}\overrightarrow{\delta x}^T \mathbf{B}^{-1}\overrightarrow{\delta x} + \frac{1}{2}\left(\vec{d} - \mathbf{HM}\overrightarrow{\delta x}\right)^T \mathbf{R}^{-1}\left(\vec{d} - \mathbf{HM}\overrightarrow{\delta x}\right)$$

Model error at the beginning of $\vec{x}_{for}$

Background model error covariance

Lin. sampling operator

Observational error covariance

GOAL DATA ASSIMILATION: find $\overrightarrow{\delta x}$ that maximizes $P(-\overrightarrow{\delta x}|\vec{o}) \leftrightarrow$ minimize J(δx)

Tangent linear model (AVRORA)

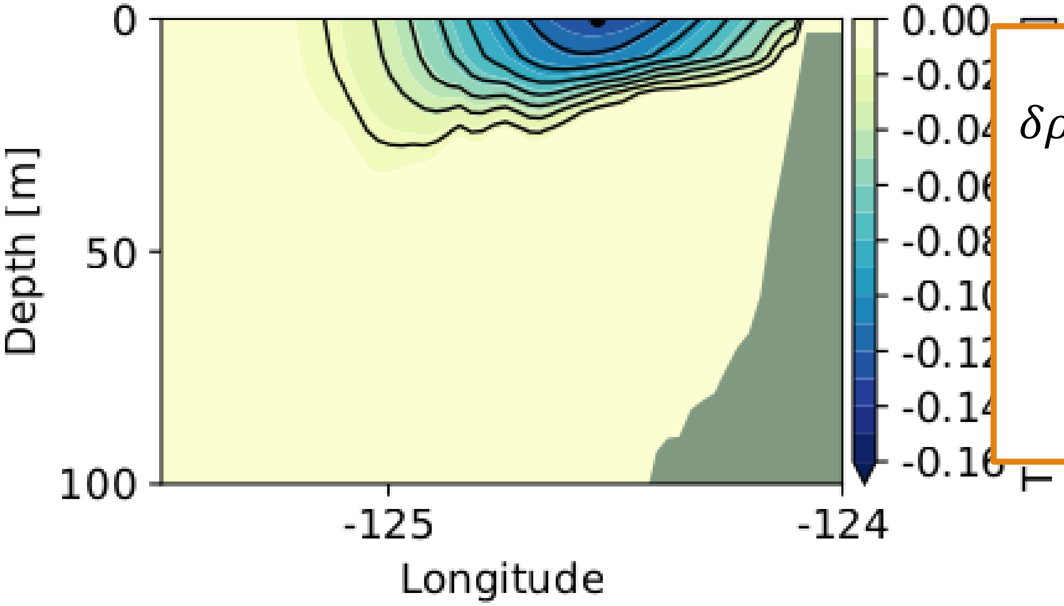
Observational error

Courtier et al., 1994: "A strategy for operational implementation of 4D-Var, using an incremental approach." *Quarterly Journal of the Royal Meteorological Societey,* 120, 1367-1387.

Model error covariance **B**

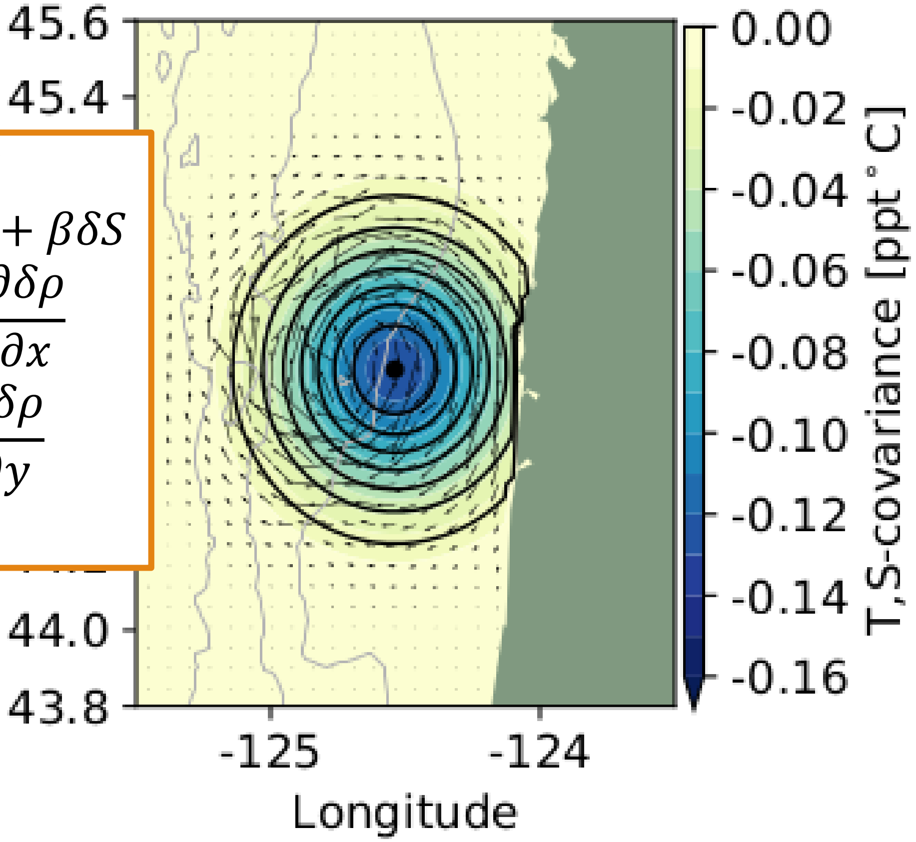
- Balance operator covariance (Weaver et al., 2005)

Temperature-salinity covariance in a zonal cross-section



$$\delta S = \gamma \delta T$$
$$\delta\rho/\rho_0 = -\alpha\delta T + \beta\delta S$$
$$\delta v = -\frac{g}{\rho_0 f}\frac{\partial\delta\rho}{\partial x}$$
$$\delta u = \frac{g}{\rho_0 f}\frac{\partial\delta\rho}{\partial y}$$

Temperature-salinity and temperature-velocity covariance at the surface



Perturbations

- Add noise $N(0,\mathbf{R})$ to observations (Houtekamer and Mitchell, 1998)
- Wind: stochastic model based around NCEI NAM fields.

$$\vec{w}_{member}(\vec{r},t) = \vec{w}_{NAM}(\vec{r},t)+\vec{w}_{Large}(\vec{r},t)+\vec{w}_{Small}(\vec{r},t)$$

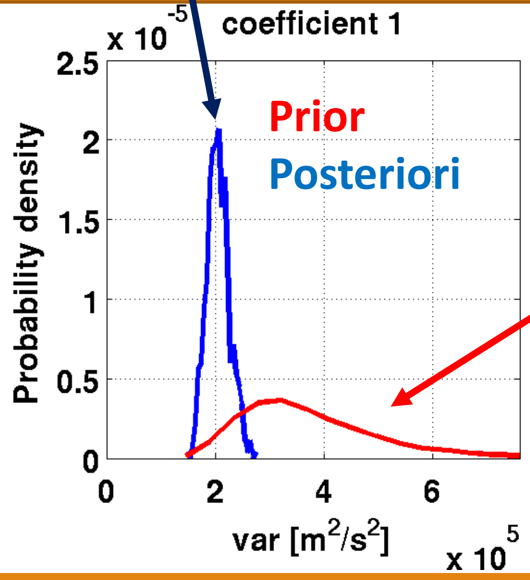
  - $\vec{w}_{NAM}$ wind from NAM model (12 km resolution)
  - $\vec{w}_{Large}(\vec{r},t)$ large scale NAM model error
  - $\vec{w}_{Small}(\vec{r},t)$ small scale NAM model error

Large-scale wind perturbations

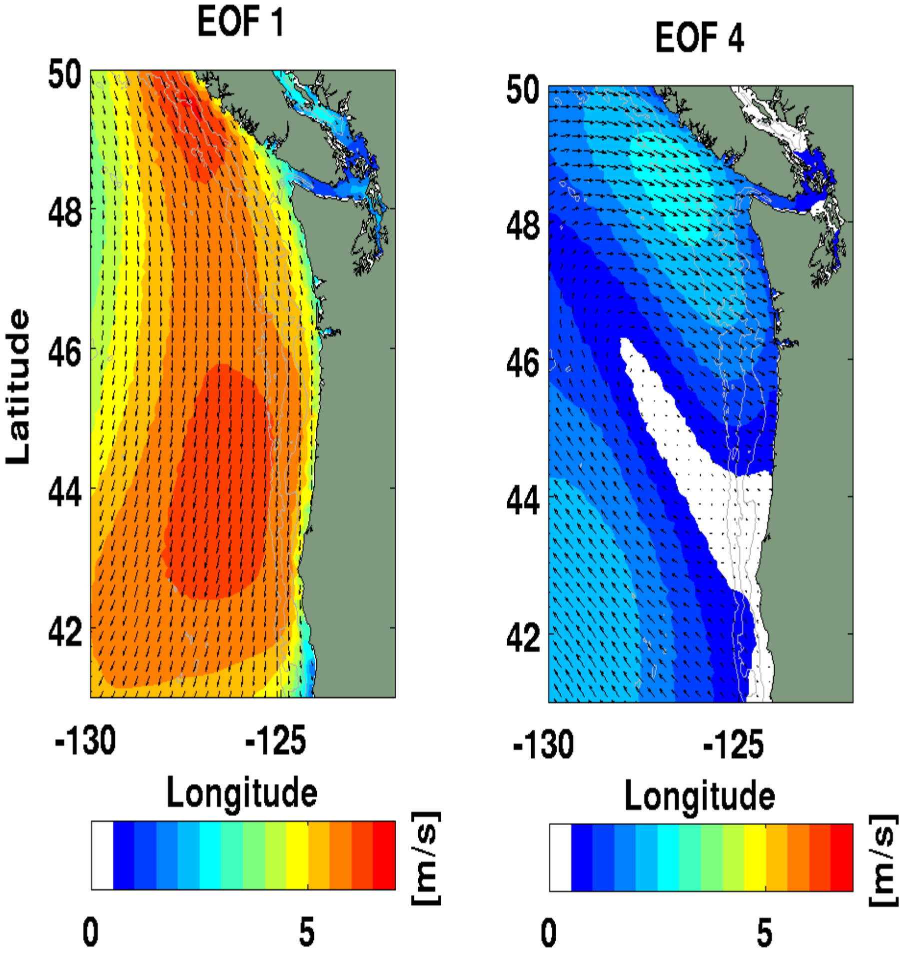
- Large scale wind perturbation:
  $\vec{w}_{Large}(\vec{r},\mathrm{t}) = \sum_{i=1}^{10} \lambda_i(t) EOF_1(\vec{r})$ $[N(\vec{\lambda};\vec{0},\vec{\sigma_L})]$
  - As e.g. Hénaff et al. (2009) with modifications
  - $\lambda_i(t)$ assumed to be drawn from AR1 process with zero mean. Correlation over 24h: 0.026
  - Standard deviation $\lambda_i(t)$ determined by applying a Gibbs sampler to error with daily ASCAT data (Milliff et al.,2011):

$$P(\vec{\lambda},\vec{w}_S,\vec{\sigma_L},\sigma_S|\vec{w}_{Ascat})\sim N(\vec{w}_{Ascat}|\vec{\lambda},\vec{w}_S,\sigma_A)N(\vec{w}_S;\vec{0},\sigma_S)IG(\sigma_S)\boldsymbol{N(\vec{\lambda};\vec{0},\vec{\sigma_L})IG(\vec{\sigma_L})}$$

Probability distribution $\sigma_{L,1},\sigma_{L,4}$



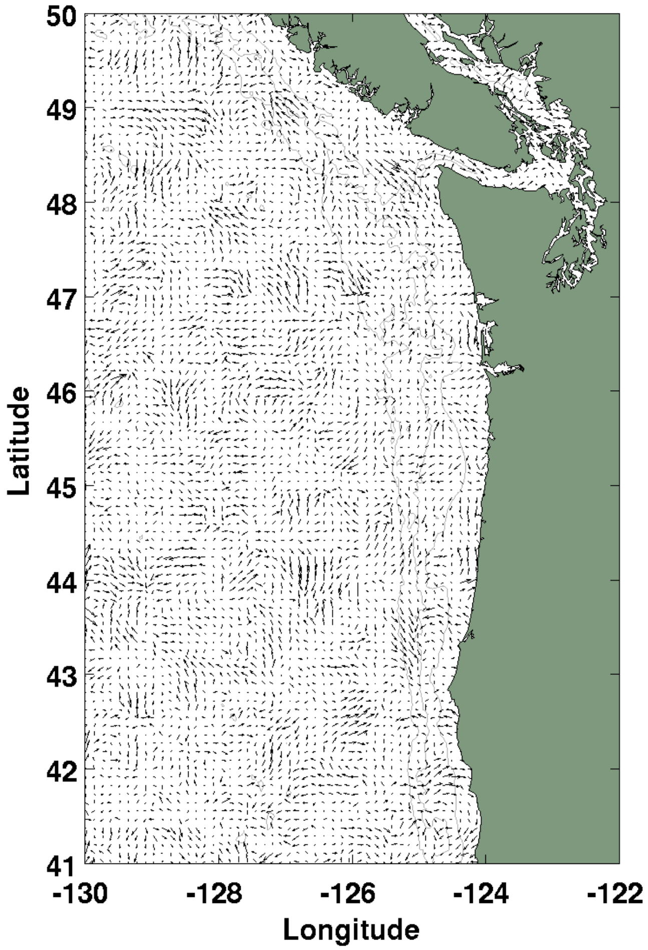
EOF wind fields



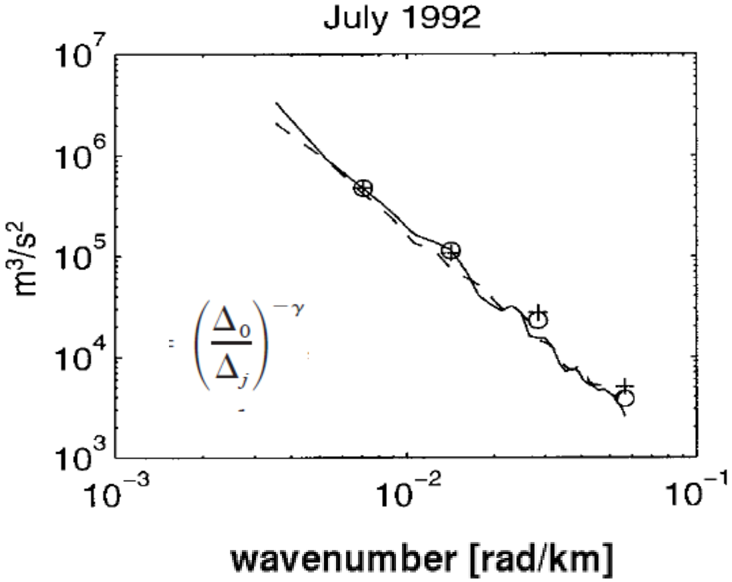
Small-scale wind perturbations

- Small scale wind perturbations:
  - Wind fields have a red spectrum
  - Linear combination of Daubechie-2 wavelets (Wikle et al.,2001) are used used to reproduce this.
  - $\vec{w}_S$ scaled such that $var(\vec{w}_S) = 2\sigma_S^2 = 1m^2s^{-2}$

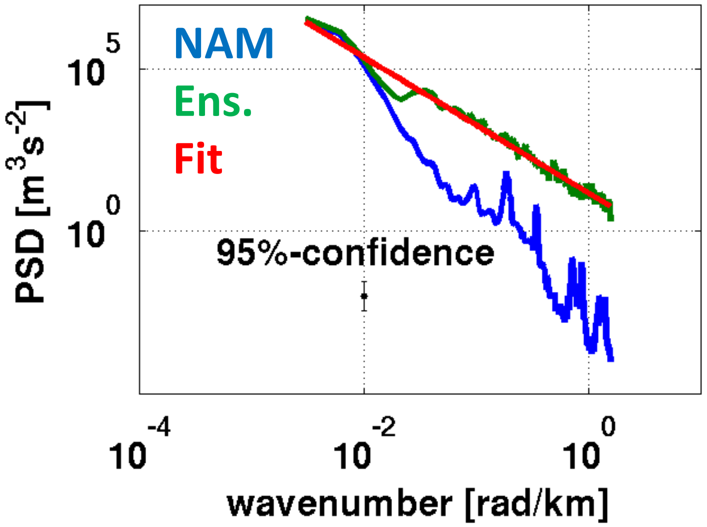
Example small-scale wind field



Spectral density of zonal (solid) and meridional (dashed) scatterometer winds (Chin et al., 1998)



Spectral density *v* in NAM and wind field ensemble members



Primal vs dual formulation

Goal: minimize J(δx) $= \frac{1}{2}\overrightarrow{\delta x}^T\mathbf{B}^{-1}\overrightarrow{\delta x} + \frac{1}{2}\left(\vec{d} - \mathbf{HM}\overrightarrow{\delta x}\right)^T\mathbf{R}^{-1}\left(\vec{d} - \mathbf{HM}\overrightarrow{\delta x}\right)$

- Primal solution:

$$(\mathbf{B}^{-1} + \mathbf{M}^T\mathbf{H}^T\mathbf{R}^{-1}\mathbf{HM})\overrightarrow{\delta x}=\mathbf{M}^T\mathbf{H}^T\mathbf{R}^{-1}\vec{d}$$

- Dual solution:

$$(\mathbf{HMB}\quad\mathbf{M}^T\mathbf{H}^T + \mathbf{R})\vec{\chi}=\vec{d},\ \overrightarrow{\delta x}=\mathbf{BM}^T\mathbf{H}^T\ \vec{\chi}$$

B: background error covariance
R: observational error covariance
M: tangent linear model
H: sampling operator
$\vec{d}$: innovation vector
$\overrightarrow{\delta x}$: 4DVAR correction
$\vec{\chi}$: solution dual

Primal vs dual formulation

- Dual solution:

  $(\mathbf{HMB}\ \ \mathbf{M}^T\mathbf{H}^T + \mathbf{R})\vec{\chi}=\vec{d},\ \overrightarrow{\delta x}=\mathbf{BM}^T\mathbf{H}^T\vec{\chi}$

- SVD preconditioned:

  Calculate random representers: $\mathbf{U\Lambda V}^{\mathrm{T}} = (\mathbf{HMB}\ \ \mathbf{M}^T\mathbf{H}^T + \mathbf{R})\boldsymbol{\Delta}$

  $\mathbf{C}^{-1/2} = \mathbf{U\Lambda}^{-1/2}\mathbf{U}^{\mathrm{T}} + (\mathbf{I}\text{-}\ \mathbf{UU}^{\mathrm{T}})$

  $\mathbf{C}^{-1/2}(\mathbf{HMB}\ \ \mathbf{M}^T\mathbf{H}^T + \mathbf{R})\mathbf{C}^{-1/2}\tilde{\chi}=\mathbf{C}^{-1/2}\vec{d},\ \overrightarrow{\delta x}=\mathbf{BM}^T\mathbf{H}^T\chi = \mathbf{BM}^T\mathbf{H}^T\mathbf{C}^{-1/2}\tilde{\chi}$

- Pro: dim($\tilde{\chi}$)<<dim($\overrightarrow{\delta x}$)
- Con: poor convergence in primal space

B: background error covariance
R: observational error covariance
M: tangent linear model
H: sampling operator
C: preconditioner
$\vec{d}$: innovation vector
$\overrightarrow{\delta x}$: 4DVAR correction
$\vec{\chi}$: solution dual

Problems E4DVAR

- Computationally challenging
  1. 4DVAR needs to applied to multiple ensemble members.
  2. 4DVAR requires multiple sequential conjugate gradient iterations to solve

$(\mathbf{R}^{-1/2}\mathbf{HMBM}^T\mathbf{H}^T\mathbf{R}^{-1/2} + \mathbf{I})\,\vec{\chi}=\mathbf{R}^{-1/2}\vec{d},\ \overrightarrow{\delta x}=\mathbf{BM}^T\mathbf{H}^T\mathbf{R}^{-1/2}\,\vec{\chi}$

$(\widetilde{\mathbf{B}} + \mathbf{I})\,\vec{\chi}=\mathbf{A}\vec{\chi} = \tilde{d},\ \overrightarrow{\delta x}=\mathbf{BM}^T\mathbf{H}^T\mathbf{R}^{-1/2}\,\vec{\chi}$

- Solution for 1:
  - Conjugate gradient minimizes[1,2] $||\vec{\chi}_i - \vec{\chi}||_{\widetilde{\mathbf{B}}\mathbf{A}}$:

$$\vec{\chi}_i = \underbrace{\mathbf{V}_{\boldsymbol{i}}(\mathbf{V}_i^T\widetilde{\mathbf{B}}\mathbf{A}\mathbf{V}_{\boldsymbol{i}})^{-1}\mathbf{V}_i^T\widetilde{\mathbf{B}}\mathbf{A}}_{\text{Projection operator}}\vec{\chi} = \mathbf{V}_{\boldsymbol{i}}(\mathbf{V}_i^T\widetilde{\mathbf{B}}\mathbf{A}\mathbf{V}_{\boldsymbol{i}})^{-1}\mathbf{V}_i^T\widetilde{\mathbf{B}}\tilde{d}$$

with $\mathrm{sp}(\mathbf{V}_{\boldsymbol{i}})$ being the Krylov space.

  - Recycle $\mathbf{V}_{\boldsymbol{i}}$: for nth ensemble member $\vec{\chi}_{n,i} = \mathbf{V}_{\boldsymbol{i}}(\mathbf{V}_i^T\widetilde{\mathbf{B}}\mathbf{A}\mathbf{V}_{\boldsymbol{i}})^{-1}\mathbf{V}_i^T\widetilde{\mathbf{B}}(\tilde{d}_{\boldsymbol{n}}+\vec{\varepsilon})$

$\vec{\varepsilon}$ is drawn from standard Gaussian. Similar Krylov space reuse, but different implementation as in EVIL[3].

B: background error covariance
R: observational error covariance
M: tangent linear model
H: sampling operator
$\vec{d}$: innovation vector
$\overrightarrow{\delta x}$: 4DVAR correction
$\vec{\chi}$: solution dual

[1]Trefethen, Lloyd N., and David Bau III. 1997. *Numerical Linear Algebra*. Vol. 50. Siam.
[2]Gurol, S., A. T. Weaver, A. M. Moore, A. Piacentini, H. G. Arango, and S. Gratton. 2014. “B-Preconditioned Minimization Algorithms for Variational Data Assimilation with the Dual Formulation.” *Quarterly Journal of the Royal Meteorological Society* 140 (679): 539–56.
[3]Auligné, Thomas, Benjamin Ménétrier, Andrew C. Lorenc, and Mark Buehner. 2016. “Ensemble–Variational Integrated Localized Data Assimilation.” *Monthly Weather Review* 144 (10): 3677–96

Parallel 4DVAR

Solution 2: expand $\mathrm{sp}(\mathbf{V}_{\boldsymbol{i}})$ with m>1 vectors per iteration.

How to find these vectors:

- Use $<\tilde{d}\tilde{d}^T> = (\widetilde{\mathbf{B}} + \mathbf{I})$ and SVD to estimate eigenvalues and eigenvector of $\widetilde{\mathbf{B}} \approx \mathbf{W\Lambda W}^{\mathrm{T}}$
- Search for linear combinations eigenvectors.
- Minimization error $||\chi - \chi_{i+1}||_{\widetilde{\mathbf{B}}\mathbf{A}} \leftrightarrow$ minimization weighted in cluster variance → K-means

$c_1\vec{w}_1 + c_2\vec{w}_2 +$ | $+c_{j-1}\vec{w}_{j-1} + c_j\vec{w}_j +$ | $+c_{N-1}\vec{w}_{N-1} + c_N\vec{w}_N$ | $= \tilde{d}_i$

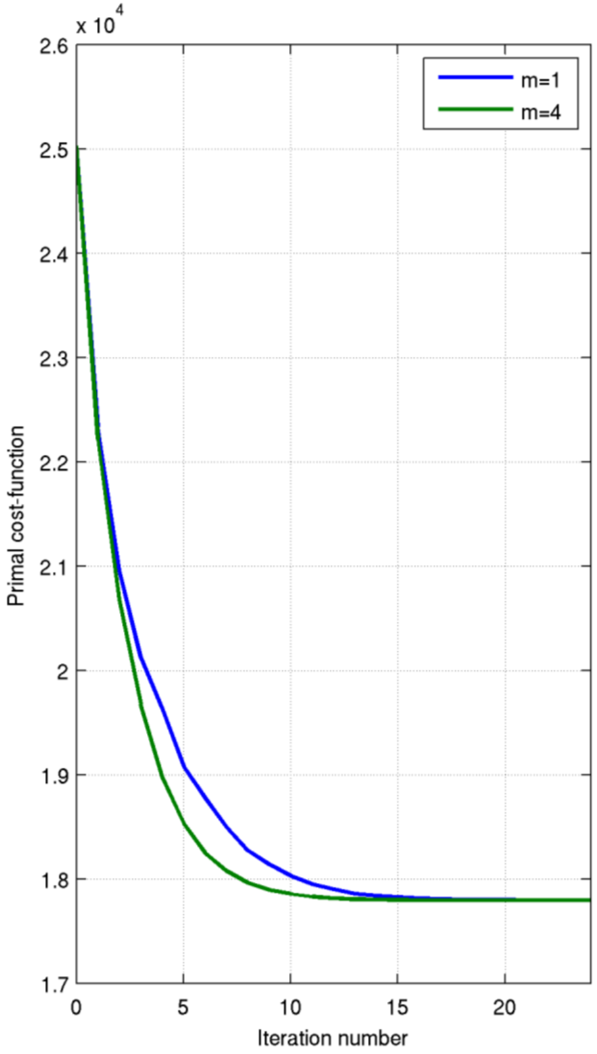
1st cluster

mth cluster

Residual previous iteration

Problems E4DVAR

- Parallel method makes minimization with less than 13 iterations feasible.



Ensemble covariance localization

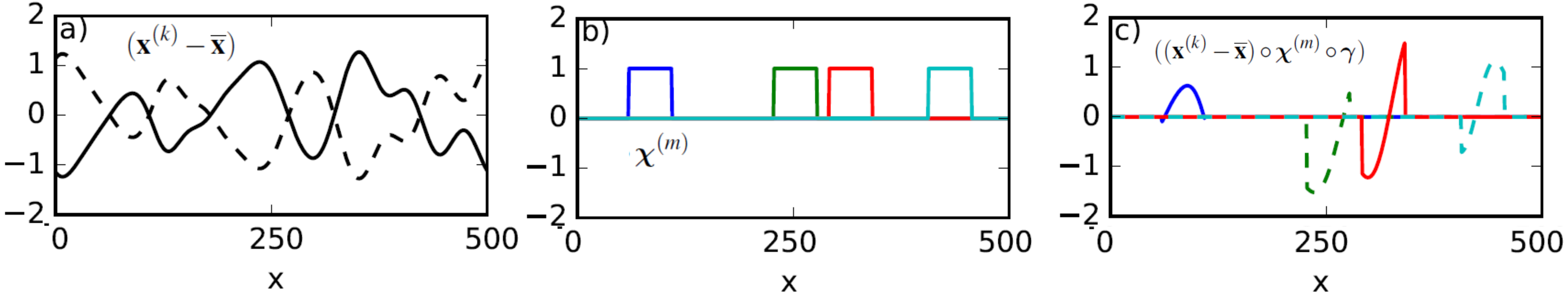
- Raw ensemble covariance: $\mathrm{B}_{ens} = \frac{1}{K-1}\sum_{k=1}^{K}(\mathbf{x}^{(k)}-\overline{\mathbf{x}})(\mathbf{x}^{(k)}-\overline{\mathbf{x}})^T$

with **x** the daily-averaged fields at the beginning of the assimilation window

B: background covariance
x: ensemble member
$\overline{\mathbf{x}}$: ensemble mean

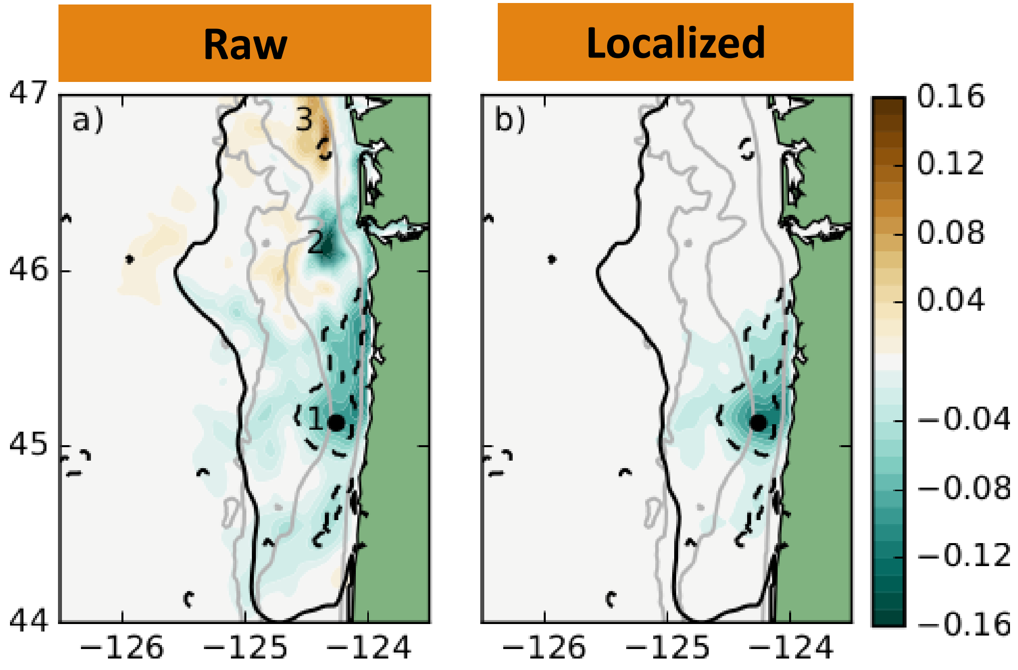
- Localized ensemble covariance using MC localization (Pasmans and Kurapov, MWR 2017 in press)

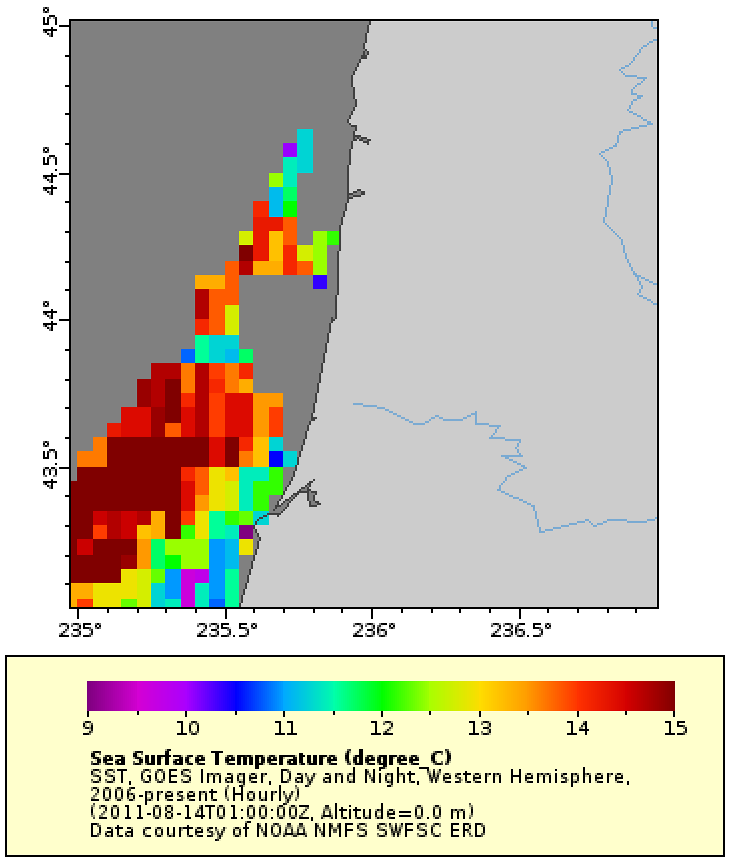
$$\mathrm{B}_{MC} = \frac{1}{K-1}\sum_{k=1}^{K}\sum_{m\in\mathbb{M}_k}((\mathbf{x}^{(k)}-\overline{\mathbf{x}})\circ\chi^{(m)}\circ\gamma)((\mathbf{x}^{(k)}-\overline{\mathbf{x}})\circ\chi^{(m)}\circ\gamma)^T, \quad \gamma_p = \left(\frac{1}{K}\sum_{k=1}^{K}\sum_{m\in\mathbb{M}_k}(\chi_p^{(m)})^2\right)^{-1/2}$$



Ensemble covariance localization

- Faster computation than Gaspari and Cohn (1999) if localization distances are comparable and number of masks < number of grid points
- Smooths spectrum ensemble members

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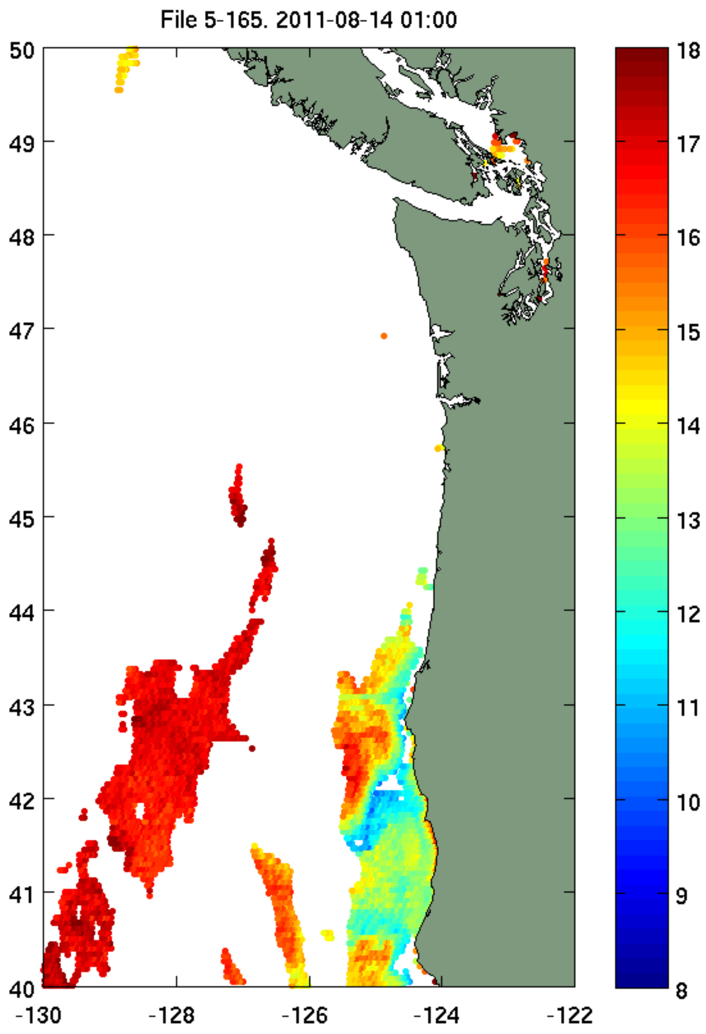
Sea Surface Temperature (degree_C)
SST, GOES Imager, Day and Night, Western Hemisphere, 2006-present (Hourly)
(2011-08-14T01:00:00Z, Altitude=0.0 m)
Data courtesy of NOAA NMFS SWFSC ERD


File 5-165. 2011-08-14 01:00
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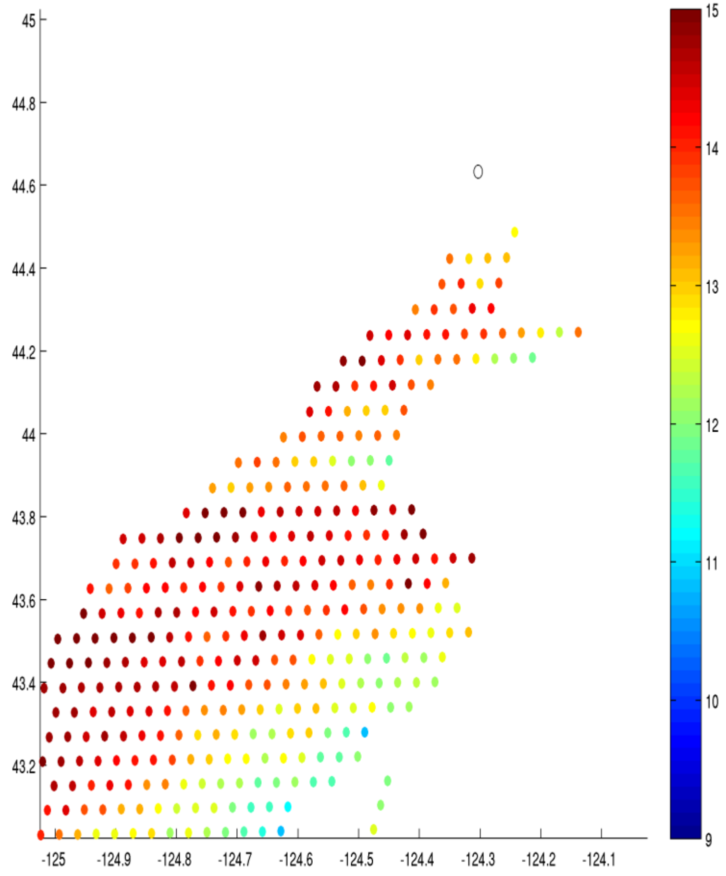
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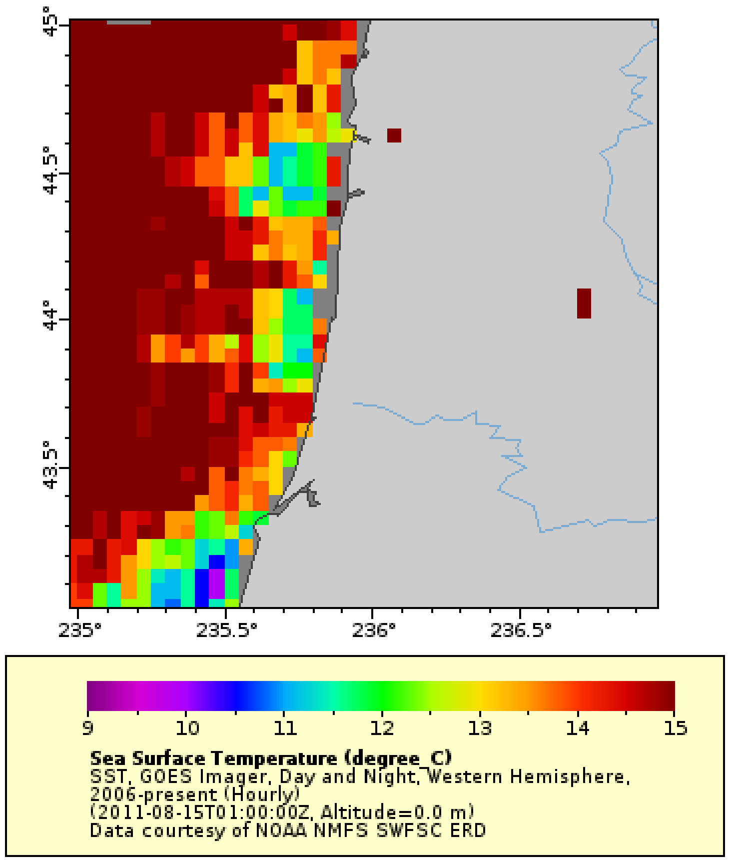
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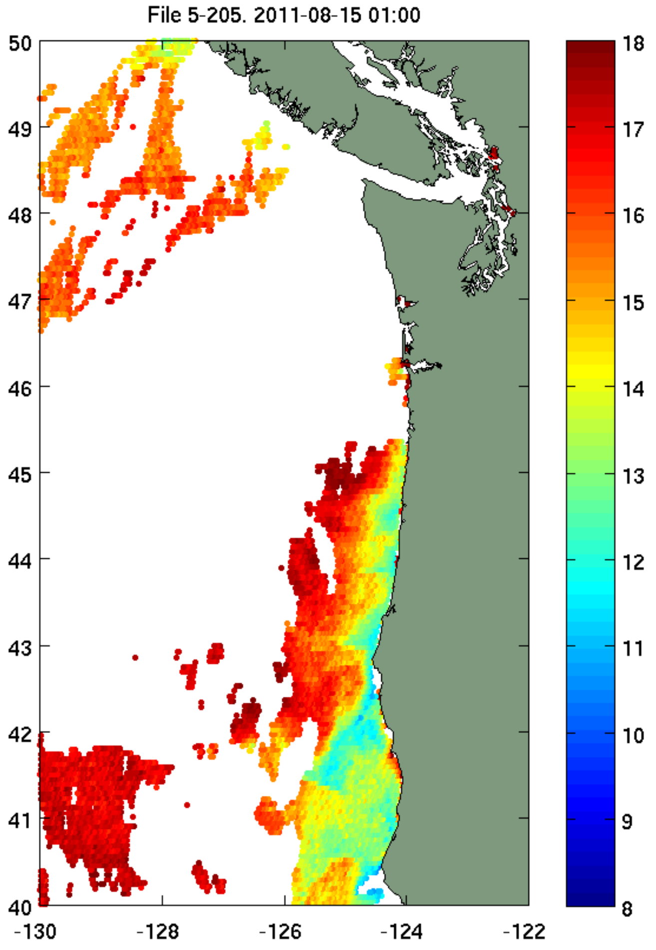
Sea Surface Temperature (degree_C)
SST, GOES Imager, Day and Night, Western Hemisphere, 2006-present (Hourly)
(2011-08-15T01:00:00Z, Altitude=0.0 m)
Data courtesy of NOAA NMFS SWFSC ERD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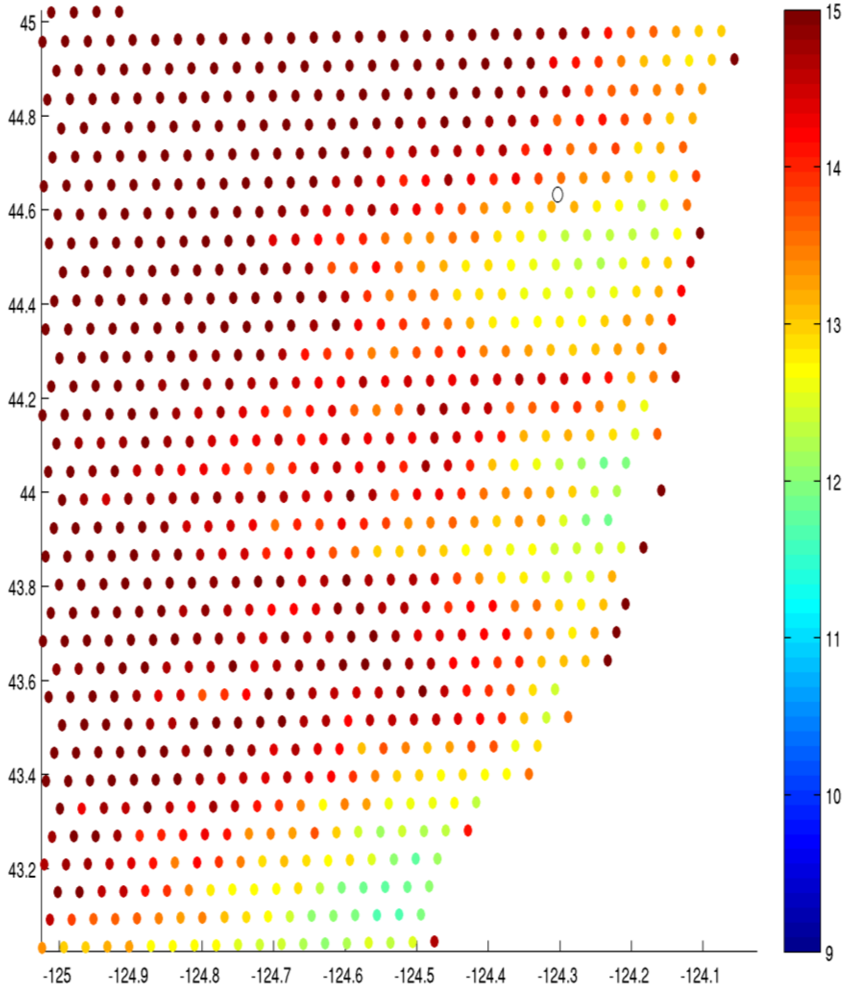
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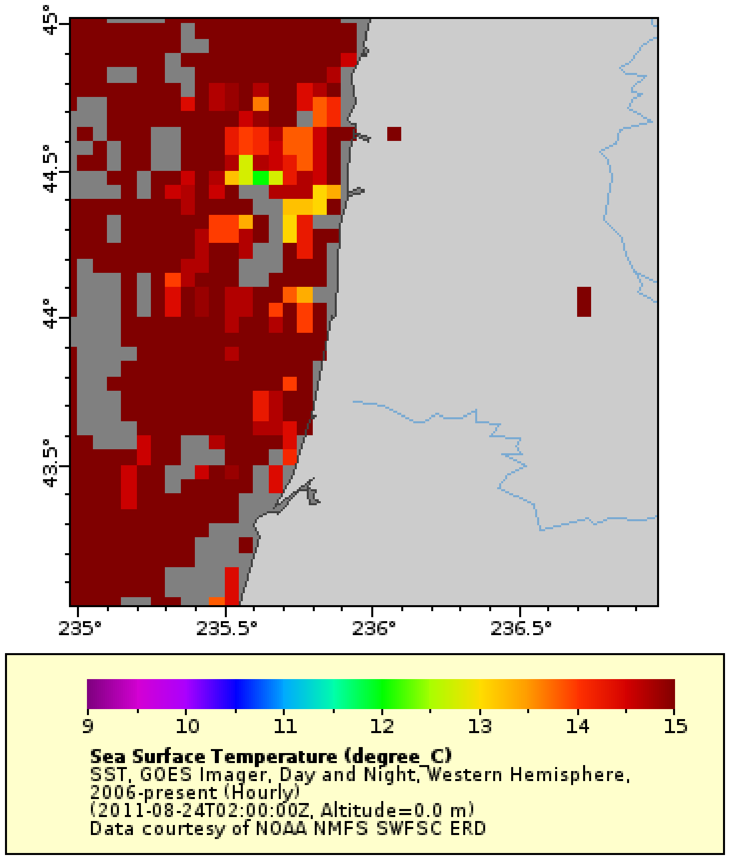
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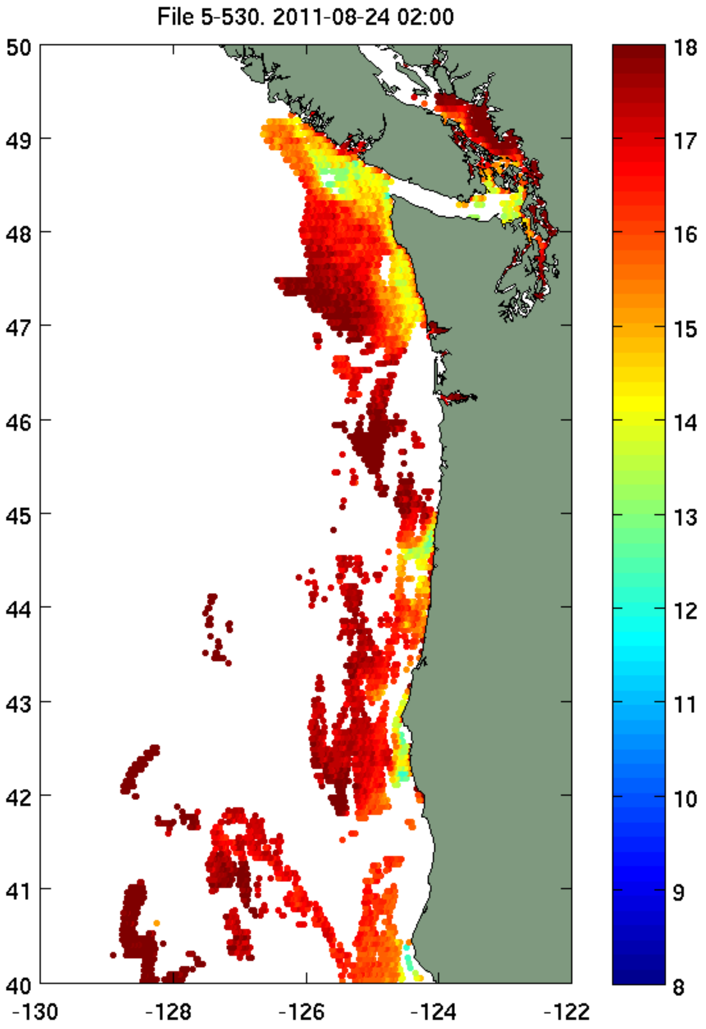
Sea Surface Temperature (degree_C)
SST, GOES Imager, Day and Night, Western Hemisphere, 2006-present (Hourly)
(2011-08-24T02:00:00Z, Altitude=0.0 m)
Data courtesy of NOAA NMFS SWFSC ERD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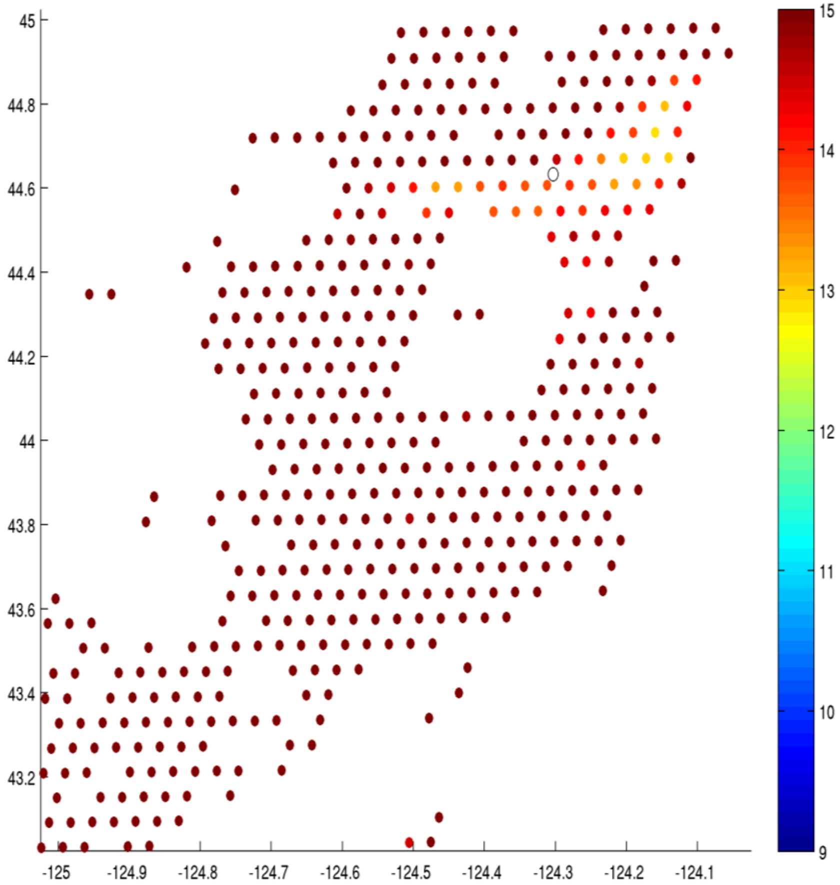
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Motivation

Forecasting of ocean conditions serves economical, safety and environmental purposes.

Fishing (photo source: amigocharters.com)

Debris tracking

Oil spill modeling (image source: Greenpeace)