# Data Assimilation at ULg

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# Outline

- Weakly constrained ensemble perturbations
- German Bight experiments (estimation of tidal boundary conditions and wind forcing using HF radar observations)
- Ligurian Sea experiments

# Improved parametrization of error covariance

- error covariance is crucial for data assimilation
- the model error covariance defines the vector space of possible model states
- ensemble method relies on perturbing model initial condition, forcing, ... within the limit of their uncertainty
- error covariance matrix $\mathbf{P} \Longleftrightarrow$ method for creating perturbations $\mathbf{x}^{(k)}$

$$\mathbf{x}^{(k)} = \mathbf{P}^{1/2}\mathbf{z}^{(k)} \qquad k \text{ ensemble index}$$

$$\mathbf{P} = E\left[\left(\mathbf{x} - E\left[\mathbf{x}\right]\right)\left(\mathbf{x} - E\left[\mathbf{x}\right]\right)^T\right]$$

- Instead of enforcing a dynamical balance as a post-processing step after the analysis, it is preferable to choose only dynamically balanced ensemble members (if possible)

# Weakly constrained ensemble perturbations

- By validation of the model with observations one can obtain an estimate of the magnitude of the perturbation.
- But which spatial structure?
- Method to create ensemble perturbation that satisfy *a priori* linear constraints
- Example of constraints:
    - geostrophic equilibrium
    - zero horizontal divergence of surface winds
    - stationary solution to the advection-diffusion equation
    - the linear shallow water equations
    - perturbations should be close to a subspace defined by *e.g.* empirical orthogonal functions (EOFs).
    - ...

# Probability of a perturbation

- To describe our *a priori* knowledge of what a realistic perturbation is, we introduce a cost function $J$, similar to the cost function used in variational analysis techniques:

$$J(\mathbf{x}) = \text{“linear balance”}^2 + \text{“smooth”}^2 + \text{“limited amplitude”}^2$$

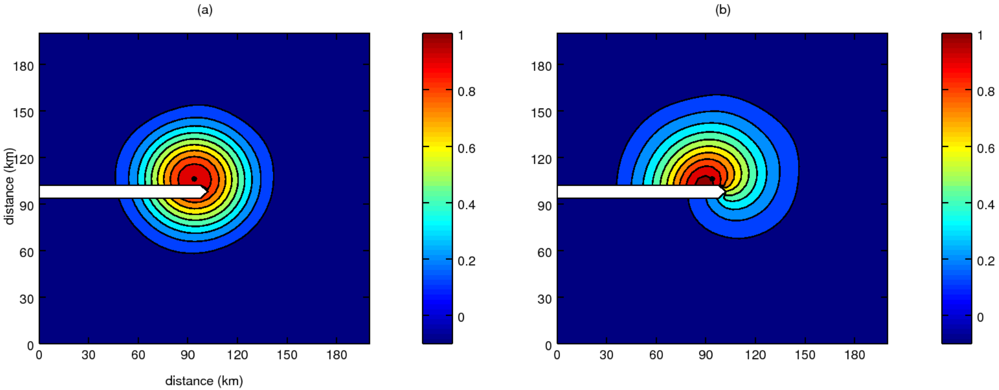
- The cost function can be used to define the probability of a perturbation $\mathbf{x}$ (*e.g.* Kalnay, 2002):

$$p(\mathbf{x}) = \alpha \exp\left(-J(\mathbf{x})\right) \tag{1}$$

- Perturbations are derived from the Hessian matrix of $J$.
- Article and source code (for MATLAB and GNU Octave) is available at `http://modb.oce.ulg.ac.be/mediawiki/index.php/WCE`

# Impact of barriers

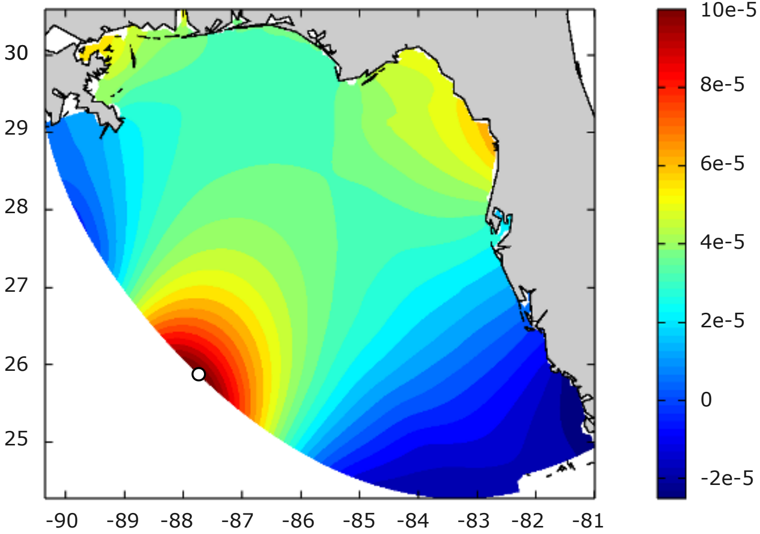
- The "smoothness" constraint is implemented through a diffusion operator (laplacian), it takes thus the land-sea mask into account




- Ensemble covariance using "classical" Fourier modes (a) and constrained perturbations based on the land-sea mask (b).

# Harmonic shallow water equations

- For tidal models, perturbations should be approximately a harmonic solution to the shallow water equations

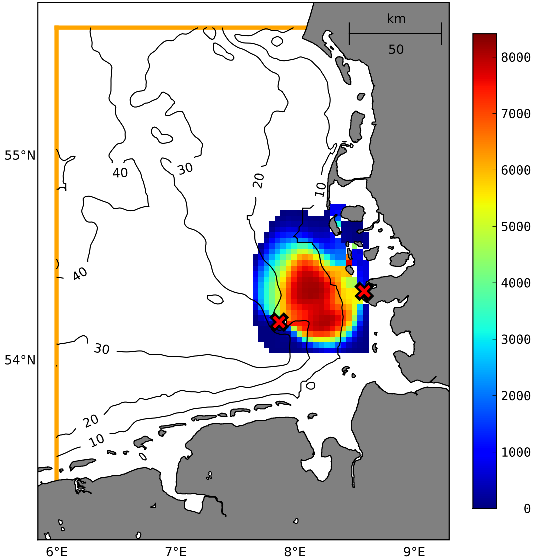



- Horizontal covariance of the constrained perturbations between the point near the open boundary marked by a black dot and all other grid points.

# German Bight model

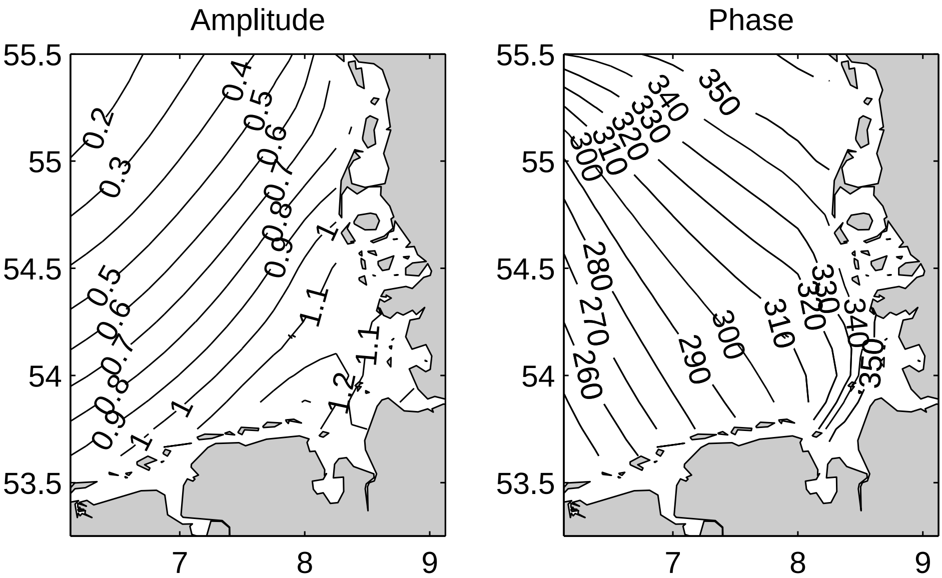
- General Estuarine Ocean Model (GETM Burchard and Bolding, 2002)
- 3-D primitive equations with a free-surface
- 21 $\sigma$ levels, resolution of about 0.9 km.
- nested in a 5-km resolution North Sea-Baltic Sea model
- ETOPO-1 topography with observations from BSH
- Atmospheric fluxes are estimated by the bulk formulation using 6-hourly ECMWF re-analysis
- Implementation by GKSS (Staneva *et al.*, 2009).

# HF radar observations

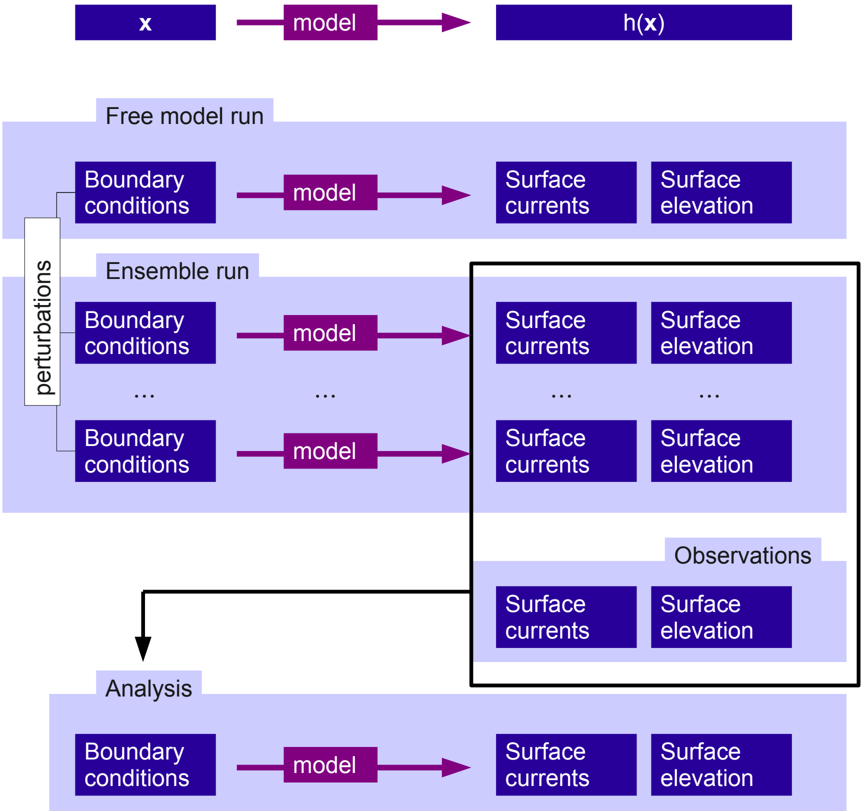



- Spatial coverage of the HF radar zonal and meridional surface velocity observations
- The number of samples available at each observation grid point is color–coded according to the color-bar.
- The crosses show the location of HF radar antennas.
- The operating frequency: 29.85 MHz (coupling to 5.02 m long ocean waves).
- HF Radar measurements from University of Hamburg (PRISMA project)

# Empirical Ocean Tides (EOT08a)




- M2 amplitude (in m) and phase (in degrees) of EOT08a for the German Bight based on altimetry.
- complex tidal parameters are assimilated


x
model
h(x)
Free model run
Boundary conditions
model
Surface currents
Surface elevation
perturbations
Ensemble run
Boundary conditions
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Surface currents
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Boundary conditions
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Surface currents
Surface elevation
Observations
Surface currents
Surface elevation
Analysis
Boundary conditions
model
Surface currents
Surface elevation

# Smoother scheme

- M2 tidal boundary conditions are perturbed within the range of their uncertainty to create a ensemble with 51 members. Perturbations are constrained by the linear shallow water equations.
- The GETM model is run for 40 days with each of those perturbed boundary values.
- All HF radar observations at any time instance within the integration period and the EOT parameters are grouped in the observation vector (vector $\mathbf{y}^o$) with their corresponding error covariance (matrix $\mathbf{R}$) estimated by cross-validation.
- The observations are extracted from every ensemble member (vector $h(\mathbf{x}^{(k)})$).
- Schematically, the non-linear operator $h(\cdot)$ performs the following operations:

$$h(\cdot) = \text{Interpolation to obs. location} \circ \text{Model integration with perturbed forcing} \tag{2}$$

# Smoother scheme

- The optimal perturbation is given the Kalman analysis (using non-linear observation operators as in Chen and Snyder (2007)):

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{A}\left(\mathbf{B}+\mathbf{R}\right)^{-1}\left(\mathbf{y}^o - h(\mathbf{x}^b)\right) \tag{3}$$

- where the matrices $\mathbf{A}$ and $\mathbf{B}$ are covariances estimated from the ensemble.

$$\mathbf{A} = \mathrm{cov}(\mathbf{x}^b, h(\mathbf{x}^b)) = \left\langle (\mathbf{x} - \langle\mathbf{x}\rangle)\left(h(\mathbf{x}) - \langle h(\mathbf{x})\rangle\right)^T \right\rangle \tag{4}$$

$$\mathbf{B} = \mathrm{cov}(h(\mathbf{x}^b), h(\mathbf{x}^b)) = \left\langle (h(\mathbf{x}) - \langle h(\mathbf{x})\rangle)\left(h(\mathbf{x}) - \langle h(\mathbf{x})\rangle\right)^T \right\rangle \tag{5}$$

where $\langle\cdot\rangle$ is the ensemble average.

- But covariance matrices do not need to be formed explicitly. Analysis is performed in the subspace defined by the ensemble members.

# Smoother scheme

- For a linear model and an infinite large ensemble, equation (14) minimizes,

$$J(x) = (\mathbf{x} - \mathbf{x}^b)^T \mathbf{P}^{b^{-1}} (\mathbf{x} - \mathbf{x}^b) + (\mathbf{y}^o - h(\mathbf{x}))^T \mathbf{R}^{-1} (\mathbf{y}^o - h(\mathbf{x})) \quad (6)$$

  or

$$J(x) = (\mathbf{x} - \mathbf{x}^b)^T \mathbf{P}^{b^{-1}} (\mathbf{x} - \mathbf{x}^b) + \sum_n (\mathbf{y}_n^o - (h(\mathbf{x})_n))^T \mathbf{R}_n{}^{-1} (\mathbf{y}_n^o - (h(\mathbf{x})_n)) \quad (7)$$

  where $n$ references to the indexed quantifies at time $n$. This is the cost function from which 4D-Var and Kalman Smoother can be derived.

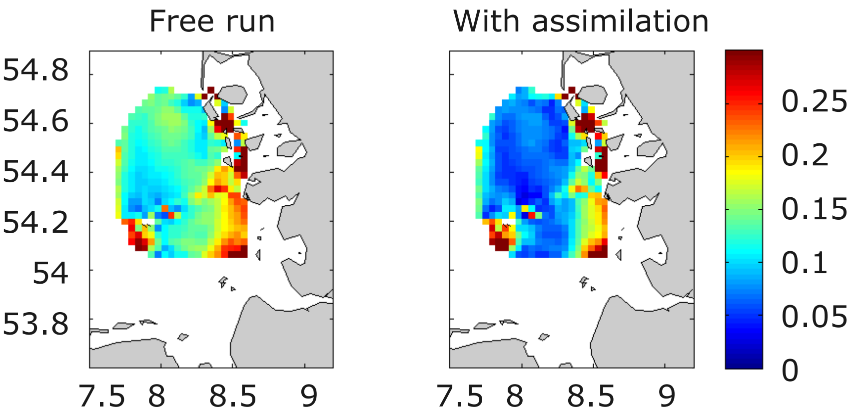
- Approach is closely related to Ensemble Smoother (van Leeuwen, 2001), 4D-EnKF (Hunt *et al.*, 2007) and AEnKF (Sakov *et al.*, 2010) where model trajectories instead of model states are optimized and to the Green's method with stochastic "search directions"

- The model is rerun with the optimized boundary values for 60 days.

# RMS difference

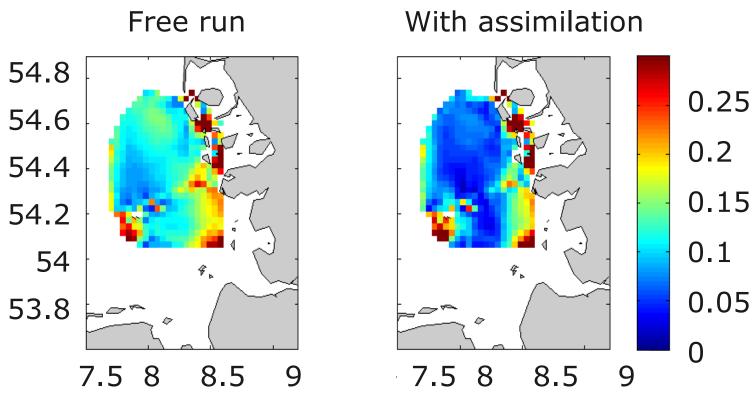
$$\text{RMS}^2 = \lim_{T\to\infty} \frac{1}{T} \int_0^T (A\cos(\omega t - \phi) - A' \cos(\omega t - \phi'))^2 dt \quad (8)$$

$$= \frac{A^2 + A'^2}{2} - AA' \cos(\phi - \phi') \quad (9)$$




RMS difference between surface current observations due to the M2 tides and the corresponding model results without (left panel) and with assimilation (right panel).

# Comparison with un-assimilated observations (M2)




- RMS difference between surface current observations (not used in the assimilation) due to the M2 tides and the corresponding model results without (left panel) and with assimilation (right panel).
- Analysis RMS compared to unassimilated data is only 0.002 m/s larger than compared to assimilated data

# Tide gage observations

| | Helgoland | | | Cuxhaven | | |
|---|---|---|---|---|---|---|
| | amplitude | phase | RMS | amplitude | phase | RMS |
| Observations | 1.13 | 304 | | 1.36 | 334 | |
| Free | 0.81 | 318 | 0.28 | 0.95 | 15 | 0.63 |
| Assimilation | 0.97 | 302 | 0.12 | 1.08 | 2 | 0.46 |

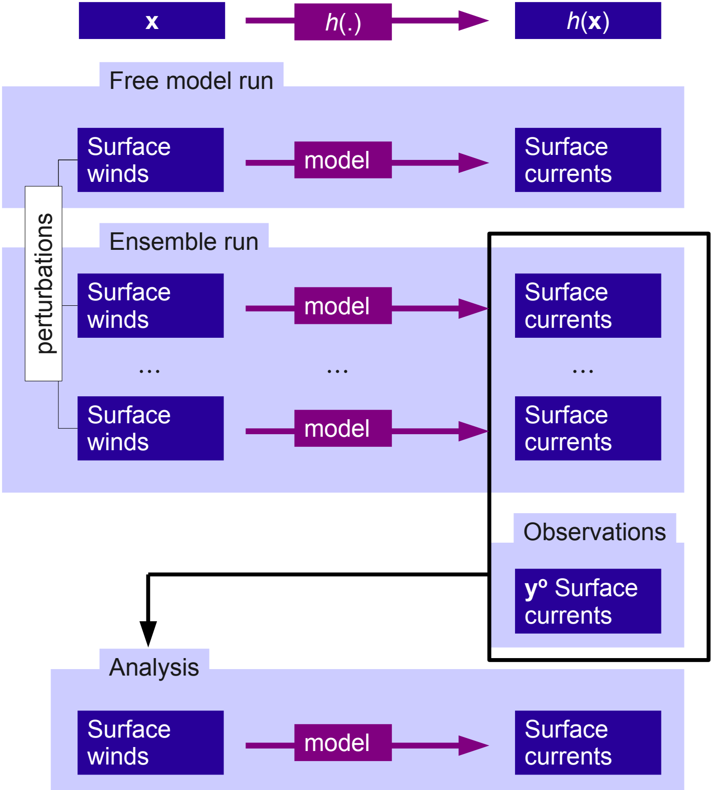
Table 1: Comparison with tide gage observations. Amplitude is in m and phase in degrees.

- Tide gage observations from different time period $\rightarrow$ only comparison of tidal parameters
- Helgoland within the area covered by radar, but not Cuxhaven
- The assimilation reduces the RMS error by a factor of 2 for Helgoland and by a factor of 1.4 for Cuxhaven.
- Ocean Science, 6, 161–178, 2010 http://www.ocean-sci.net/6/161/2010/os-6-161-2010.pdf.

# Wind estimation from HF radar observations

- Ensemble of 100 wind forcings are created (by using a Fourier decomposition)
- estimation vector $\mathbf{x}$: u- and v- component of wind forcing
- observations: $\mathbf{y}^o$: surface currents
- "observation operator" $h(\cdot)$:

$$h(\cdot) = \text{Interpolation to obs. location} \circ \text{Model integration with perturbed wind} \tag{10}$$



x
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Free model run
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perturbations
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Analysis
Surface winds
model
Surface currents

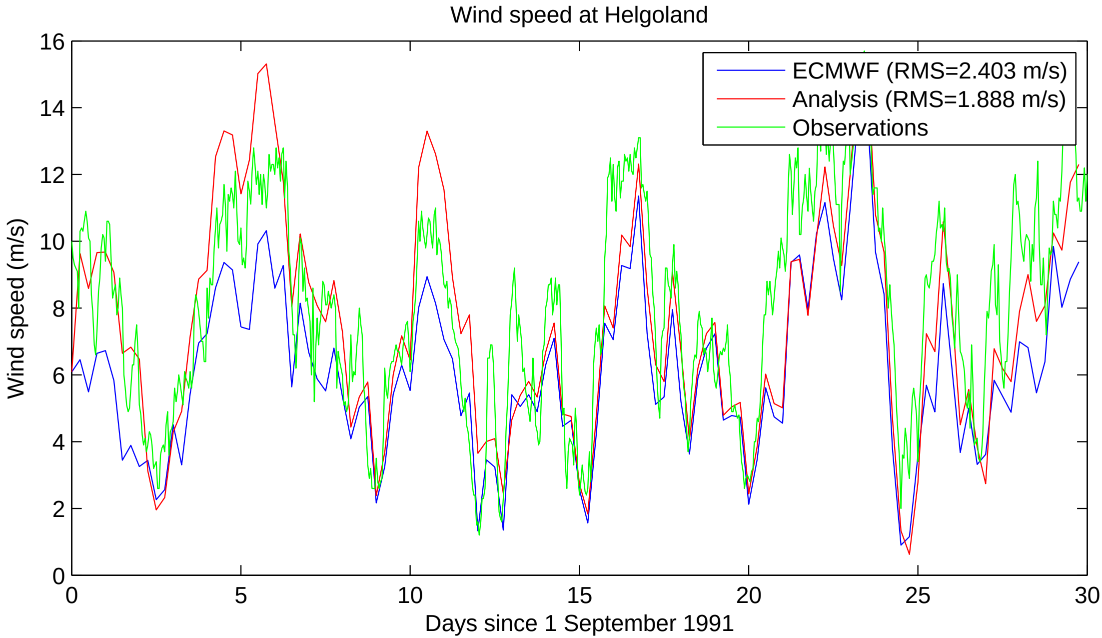



Figure 1: Measured wind speed, wind speed from ECMWF and analyzed wind speed at Helgoland. Units are m/s.

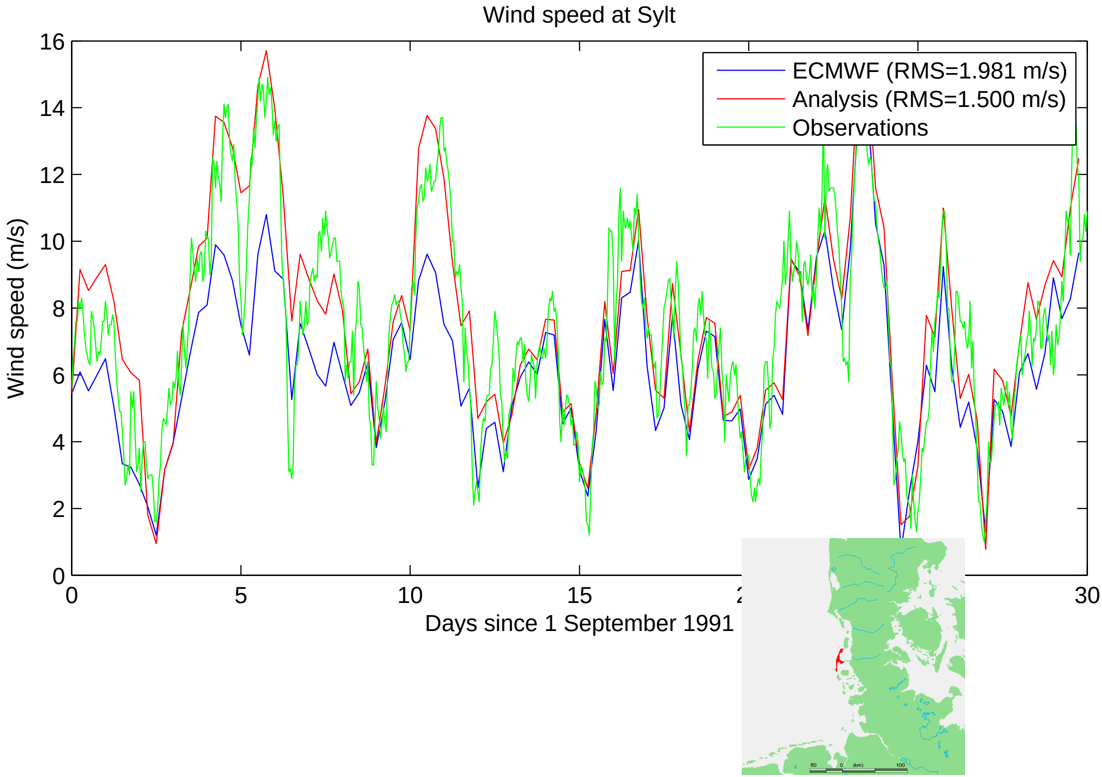



Figure 2: Measured wind speed, wind speed from ECMWF and analyzed wind speed at Sylt. Units are m/s.

# Comparison with satellite SST

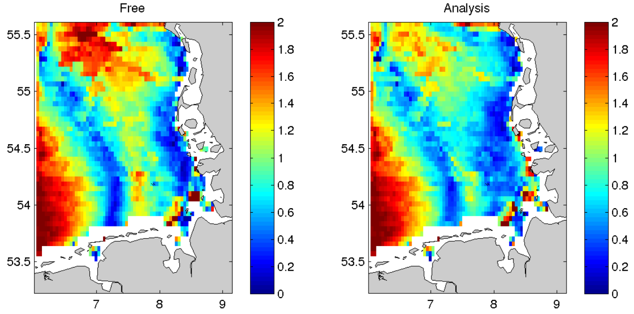


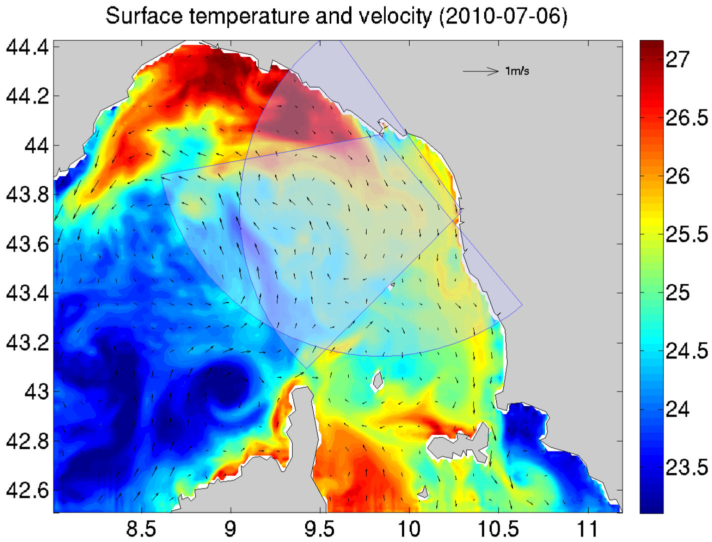

Figure 3: RMS difference between AVHRR SST and model SST without assimilation (left panel) and with assimilation (right panel)

| | $S_{\mathrm{HF}}$ | RMS | skill score |
|---|---|---|---|
| Free | – | 1.21 | 0.00 |
| Analysis | 0.5 | 1.09 | 0.19 |
| | 1.0 | 1.09 | 0.19 |
| | 1.5 | 1.10 | 0.18 |
| | 2.0 | 1.11 | 0.16 |
| | 2.5 | 1.12 | 0.14 |
| | 5.0 | 1.16 | 0.08 |

RMS is expressed in °C and $S_{\mathrm{HF}}$ in m/s.

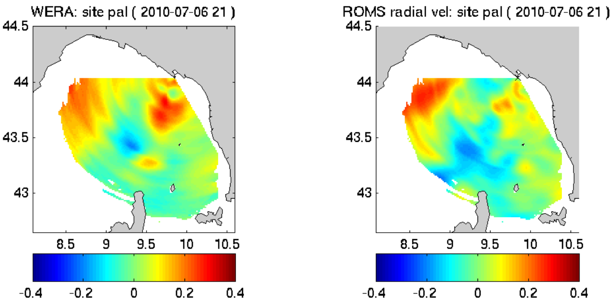
# Ligurian Sea Model (WP5)

- ROMS nested in Mediterranean Ocean Forecasting System
- 1/60 degree resolution and 32 vertical levels
- Currents: Western & Eastern Corsican Current, Northern Current, inertial oscillation
- Two WERA HF radar systems (Palmaria, San Rossore) by NATO Undersea Research Centre (NURC)



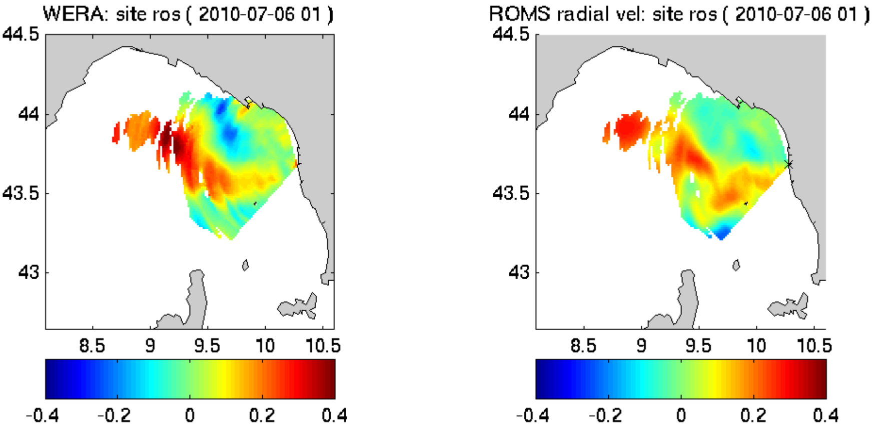

# Observations

- Frequency of $\nu = 12.359$ MHz and coupled to a wave length of $\lambda_b = 12.13$ m,
- Radial currents are used for the assimilation
- Azimuthal resolution of 6 degrees
- Currents are averaged over 1 h




Radial currents on 2010-07-06 21:30 relative to the Palmaria site: left panel shows WERA measurements and right panel shows ROMS results without assimilation.

# Observations




Radial currents on 2010-07-06 01:30 relative to the San Rossore site: left panel shows WERA measurements and right panel shows ROMS results without assimilation.

# Observation operator

- Radial currents are extracted by:

$$u_{\mathrm{HF}} = \frac{k_b}{1 - \exp(-k_b h)} \int_{-h}^{0} \mathbf{u}(z) \cdot \mathbf{e}_r \exp(k_b z) dz \tag{11}$$

  - $k_b = \frac{2\pi}{\lambda_b}$
  - $\mathbf{e}_r$ is the unit vector pointing in the direction opposite to the location of the HF radar site
  - positive values: current away from the system
  - essentially represent an average over the upper meters.
- Smoothed in the azimuthal direction by a diffusion operator to filter scales smaller than 6 degrees

# Model errors covariance

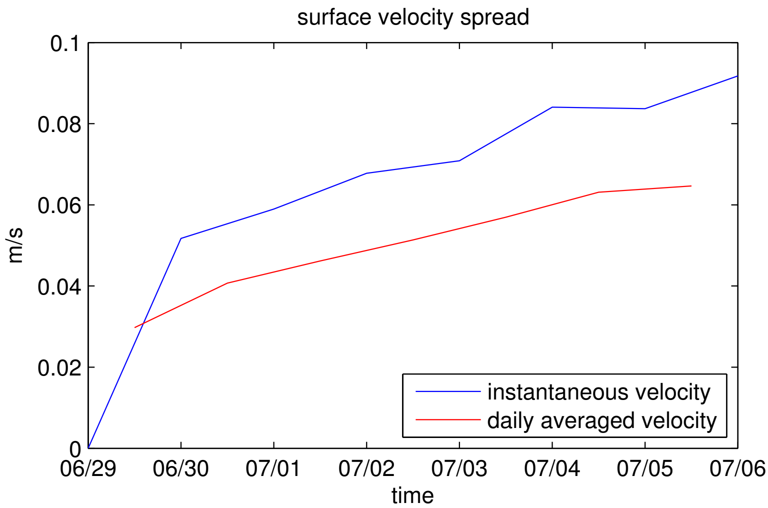
- Estimated by ensemble simulation where uncertain aspect of the model are perturbed
- Perturbed zonal and meridional wind forcing
- Perturbed boundary conditions (elevation, velocity, temperature and salinity)
- Perturbed momentum equation ($\varepsilon$)

$$\frac{d\mathbf{u}}{dt} + \mathbf{\Omega} \wedge \mathbf{u} = -\frac{1}{\rho_0}\nabla_h p + \frac{1}{\rho_0}\nabla \cdot \mathbf{F}^{\mathbf{u}} + \nabla_h \wedge \ \varepsilon \, \mathbf{e}_z \tag{12}$$

$$\tag{13}$$

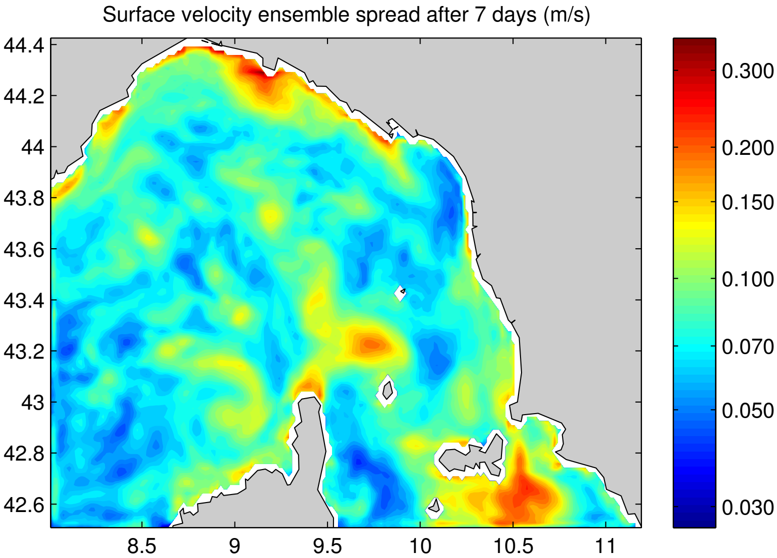
- where $\nabla_h = \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y}$
- does not create horizontal convergence or divergence (linked to barotropic waves)
- can create mesoscale flow structures (absent or misplaced)

# Ensemble spin-up



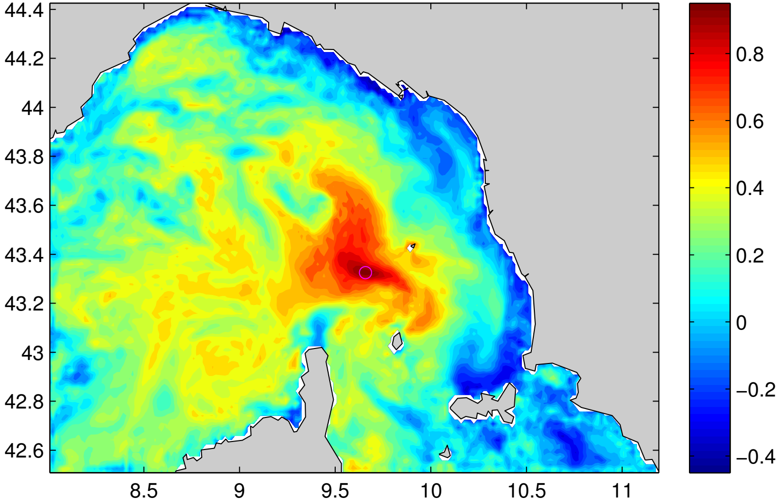

- Ensemble of IC is created by a 7 day ensemble integration starting from the same IC but with perturbed forcing (ensemble spin-up)
- Spin-up should create mesoscale circulation features

# Velocity spread



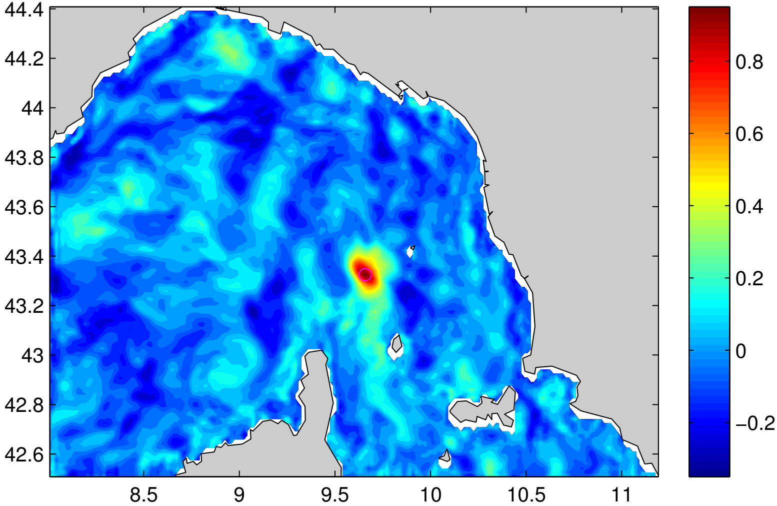

- Velocity spread after 7 days
- Largest uncertainties near eddies

# Spatial correlation



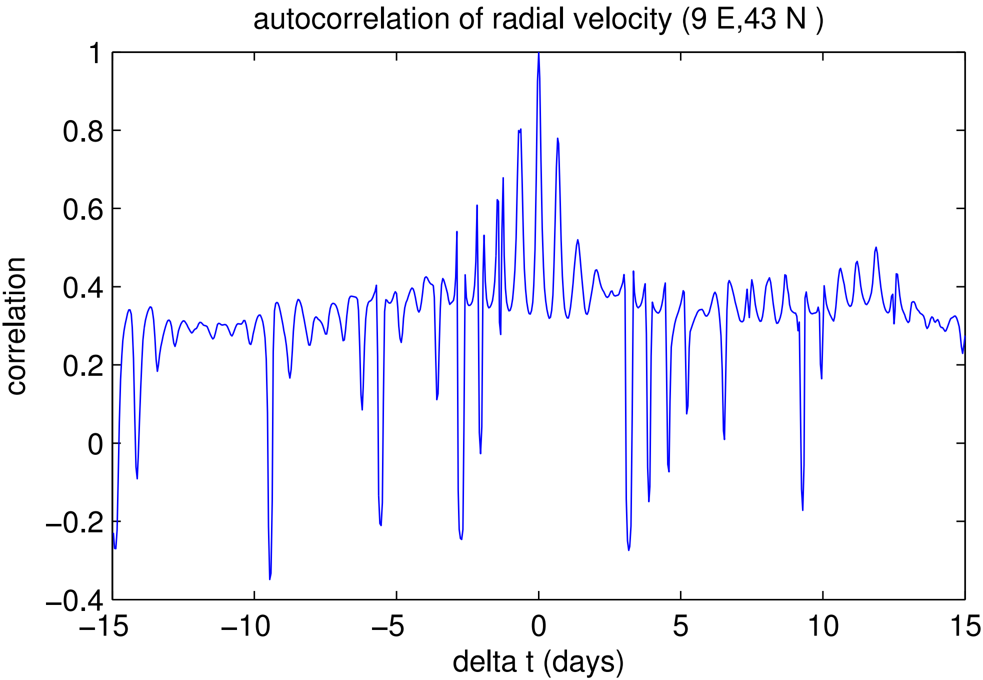

- Correlation of temperature at a specific point (magenta circle) and other surface grid points
- Resulting length-scale is about 50 km

# Spatial correlation




- Correlation of zonal velocity at a specific point (magenta circle) and other surface grid points
- Resulting length-scale is about 10 km
- Adequately observing surface velocity would require measurements with higher spatial resolution that the resolution of temperature measurements

## Temporal correlation




periodicity of 16 h (period of inertial oscillations is 17.6 h)

# Data assimilation scheme

- Time dimension embedded in estimation vector $\mathbf{x}$
- Different definitions of estimation vector are possible:
  - $\mathbf{x} =$ (model trajectory), *i.e.* model state at all time instances
  - $\mathbf{x} =$ (uncertain forcing fields), here IC, BC, wind and stochastic error term at all time instances
  - $\mathbf{x} =$ (model trajectory, uncertain forcing fields)
- The optimal $\mathbf{x}$ is given by the Kalman analysis (using non-linear observation operators as in Chen and Snyder (2007)):

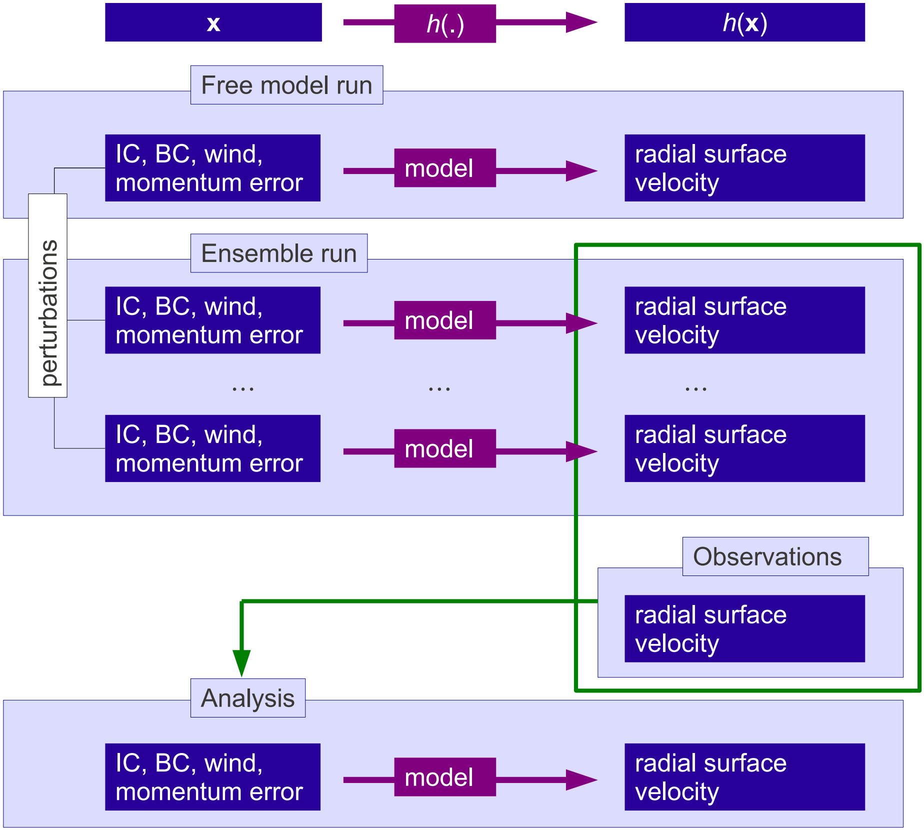
$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{A}\left(\mathbf{B}+\mathbf{R}\right)^{-1}\left(\mathbf{y}^o - h(\mathbf{x}^b)\right) \tag{14}$$

- where the matrices $\mathbf{A}$ and $\mathbf{B}$ are covariances estimated from the ensemble.

$$\mathbf{A} = \mathrm{cov}(\mathbf{x}^b, h(\mathbf{x}^b)) = \left\langle \left(\mathbf{x} - \langle\mathbf{x}\rangle\right)\left(h(\mathbf{x}) - \langle h(\mathbf{x})\rangle\right)^T \right\rangle \tag{15}$$

$$\mathbf{B} = \mathrm{cov}(h(\mathbf{x}^b), h(\mathbf{x}^b)) = \left\langle \left(h(\mathbf{x}) - \langle h(\mathbf{x})\rangle\right)\left(h(\mathbf{x}) - \langle h(\mathbf{x})\rangle\right)^T \right\rangle \tag{16}$$

where $\langle\cdot\rangle$ is the ensemble average.


x
h(.)
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Free model run
IC, BC, wind, momentum error
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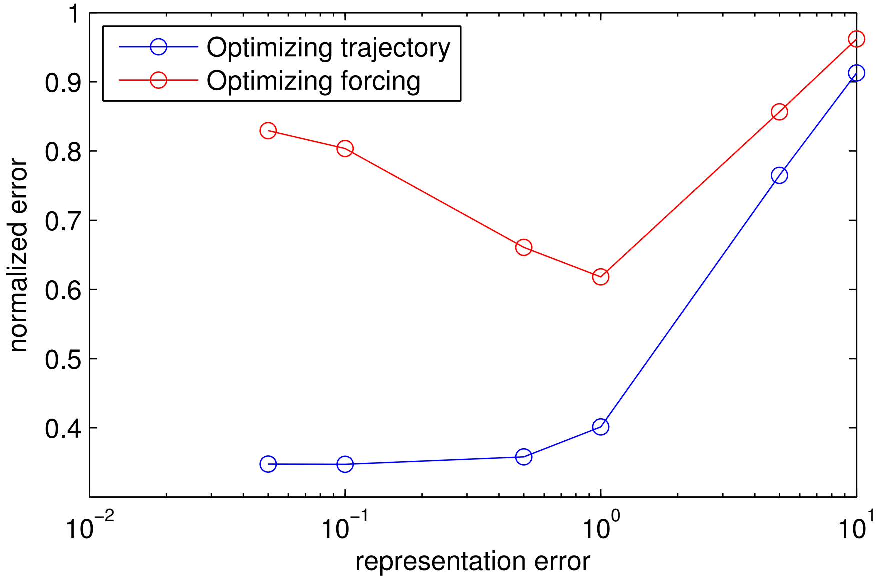
IC, BC, wind, momentum error
model
radial surface velocity
Observations
radial surface velocity
Analysis
IC, BC, wind, momentum error
model
radial surface velocity

## Estimation of trajectory versus estimation of forcing fields

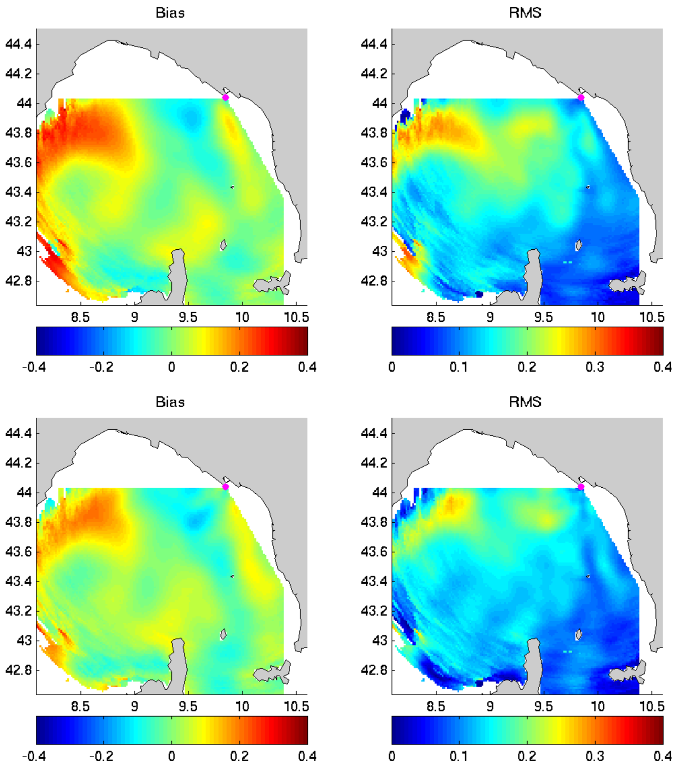



- Both approaches equivalent for linear system (and additive noise)
- Unrealistic "ensemble extrapolation" when too small observation errors are used $\rightarrow$ model trajectory and forcing fields are inconsistent

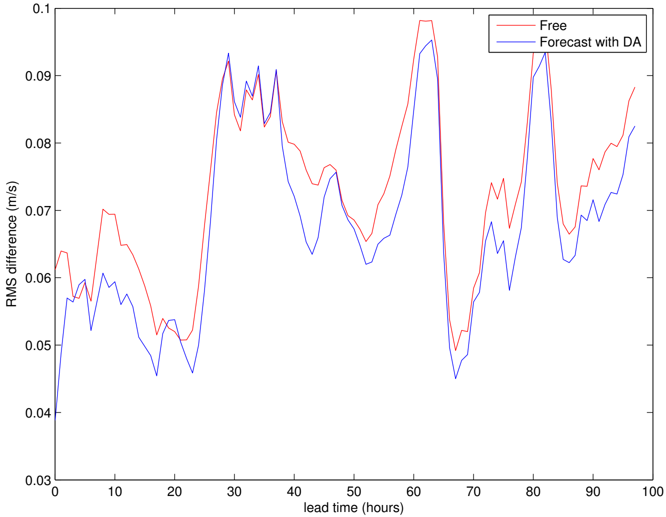
# Error statistics for Palmaria Site

Without assimilation (positive values: current away from the magenta dot)

With assimilation



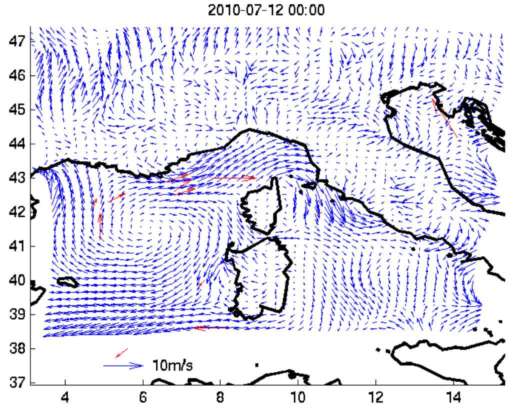
# Forecasts




- Impact of data assimilation on current forecast
- Comparison with surface currents from Palmaria
- HF radar assimilation improves the strength of the Northern Current and this improvement persists for some time.

# Simulation with atmospheric model (WRF)

- blue arrows: WRF 10m wind vectors, red arrows: in situ wind measurements from ICOADS (International Comprehensive Ocean-Atmosphere Data Set).wind_LS2.mp4
- 3 WRF domains at 30, 10, 3.33 km resolution (two-way nesting). The limit of those domains are shown in black.
- 30-km grid model nested (one-way) into the Global Forecast System
- 28 vertical layers



# Model results with different wind forcings

- Total RMS differences (m/s):

| | Pal. | Ros. |
|---|---|---|
| COSMO | 0.14 | 0.11 |
| WRF | 0.13 | 0.14 |

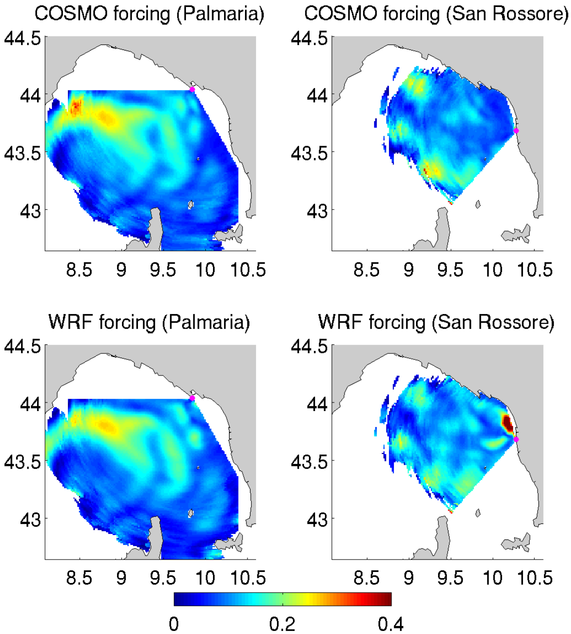



Figure 4: Radial surface current RMS difference

# Ocean Assimilation Kit

- Reduced rank square root analysis
- Global and local algorithm
- Modular Fortran 90 program
- Flexible definition of state vector
- Supports arbitrary curvilinear grid
- Local algorithm parallelized with OpenMP and MPI
- NetCDF or Fortran binary files as input

```
Model.variables = [                  'zeta',          'temp',         'salt']
Model.gridX     = ['domain.nc#lon(:,:,end)','domain.nc#lon','domain.nc#lon']
Model.gridY     = ['domain.nc#lat(:,:,end)','domain.nc#lat','domain.nc#lat']
Model.gridZ     = [  'domain.nc#z(:,:,end)',  'domain.nc#z',  'domain.nc#z']
Model.mask      = [  'domain.nc#z(:,:,end)',  'domain.nc#z',  'domain.nc#z']
Model.path      = '/home/user/Data/'

Syntax:
NetCDF_filename.nc#NetCDF_variable(index list)
```

# Ocean Assimilation Kit - Observations

```
Obs001.time       = '2010-07-06T00:30:00.00'  ! time as YYYY-MM-DDThh:mm:ss
Obs001.path       = 'Obs/'                     ! where the file can be found
Obs001.variables  = [               'TEM']    ! name as in Model.variables
Obs001.names      = [      'temp_profile']    ! descriptive name
Obs001.gridX      = [       'obs1.nc#lon']    ! longitude
Obs001.gridY      = [       'obs1.nc#lat']    ! latitude
Obs001.gridZ      = [         'obs1.nc#z']    ! depth
Obs001.value      = [      'obs1.nc#temp']    ! value of the observations
Obs001.mask       = [      'obs1.nc#temp']    ! mask of the observations
Obs001.rmse       = [ 'obs1.nc#temp_rmse']    ! root mean square error
```

# Implementation

Compact algorithm using Fortran operators:

```
Hxf = H.x.xf
increment = Sf.x.(U.x.(lambda.dx.(U.tx.(HSf.tx.(invsqrtR**2*(yo-Hxf))))))
```

Definition of operators .x., .tx., .dx and sparse matrix type H

# Conclusions

- Ensemble assimilation methods require realistic perturbation schemes (error co-variances) which can be based on dynamical relationships (similar to Variational analysis)
- Tidal boundary conditions can be constrained by HF radar measurements.
- Correcting tidal boundary conditions avoids (or at least reduces) systematic errors in the model solution.
- Similar approach can also be used to adjust wind forcings using HF radar data.
- Embedding the time dimension into the state vector leads to a smoother scheme (which is very simple to implement)
- Smoother schemes can be used to estimate the optimal model trajectory or forcing field
- Both approaches are not equivalent for non-linear systems or multiplicative noise

# References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# Perturbations scheme

The cost function is a quadratic function in $\mathbf{x}$ and can thus be written as:

$$
\begin{aligned}
2J(\mathbf{x}) &= \mathbf{x}^T(\mathbf{M}^T\mathbf{W}_M\mathbf{M} + \mathbf{D}^T\mathbf{W}_D\mathbf{D} + \mathbf{W}_E)\mathbf{x} \qquad (17)\\
&= \mathbf{x}^T\mathbf{B}^{-1}\mathbf{x} \qquad (18)
\end{aligned}
$$

where the matrix $\mathbf{B}$ (covariance matrix, not formed explicitly) is defined as:

$$\mathbf{B} = (\mathbf{M}^T \mathbf{W}_M \mathbf{M} + \mathbf{D}^T \mathbf{W}_D \mathbf{D} + \mathbf{W}_E)^{-1} \tag{19}$$

To generate an ensemble of perturbations that follows the previous pdf, the matrix $\mathbf{B}$ is decomposed in eigenvectors (rows of $\mathbf{U}$) and eigenvalues (diagonal elements of $\mathbf{\Lambda}$) :

$$\mathbf{B} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T \tag{20}$$

The smaller an eigenvalue is, the stronger the corresponding eigenvector violates the dynamical and smoothness constraint.

An ensemble of vectors $\mathbf{z}^{(k)}$ where the subscript $k$ is the ensemble member, is created following a normal distribution.

$$\mathbf{z} \sim N(0, \mathbf{I}_n) \tag{21}$$

An ensemble of perturbations $\mathbf{x}^{(k)}$ following (1) can be obtained by:

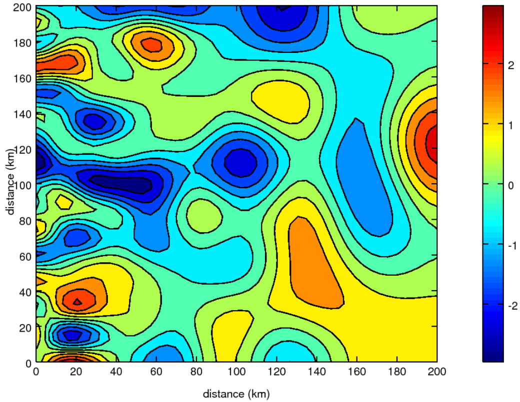
$$\mathbf{x}^{(k)} = \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{z}^{(k)} \tag{22}$$

Alternatively, one can use the 2nd order exact re-sampling method (SEIK):

$$\mathbf{x}^{(k)} = \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{H}_w(\Omega)_k \tag{23}$$

where columns of $\mathbf{H}_w$ are all perpendicular to the vector $\mathbf{1}_{N\times 1}$ and $(\Omega)_k$ is the $k$-column of a random orthogonal matrix $\Omega$.

- Also perturbations with a spatially varying correlation length can be created.
- Scale of mesoscale variability $\rightarrow$ internal radius of deformation which varies in space:



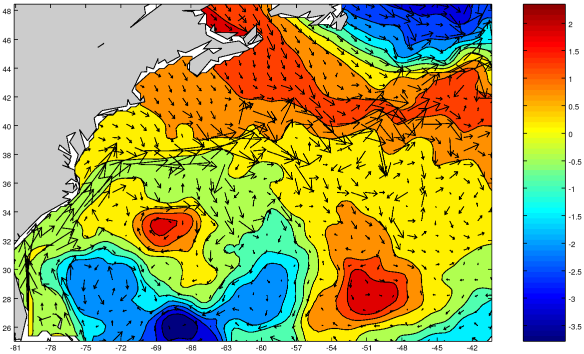

- Illustration of a random field with a variable correlation length.

# Examples for linear constraints

## Advection constraint

- For large-scale models, perturbations should be approximately stationary solutions to the advection equation

$$\mathbf{v} \cdot \nabla \phi = 0 \tag{24}$$



- Example of ensemble perturbations using the advection constraint

# Application to HF Radar assimilation in the German Bight (tidal BC)

- Only M2 tidal boundary conditions are perturbed:

$$\zeta^{(k)} = \zeta^{(b)} + \Re\left(\zeta'(x,y)\exp(i\omega t)\right) \tag{25}$$

where $\omega$ is the M2 angular frequency and $\zeta'(x,y)$ is a random field satisfying approximately the harmonic shallow water equations:

$$i\omega\zeta' + \frac{\partial(hu')}{\partial x} + \frac{\partial(hv')}{\partial y} = 0 \tag{26}$$

$$i\omega u' - fv' + g\frac{\partial \zeta'}{\partial x} = 0 \tag{27}$$

$$i\omega v' + fu' + g\frac{\partial \zeta'}{\partial y} = 0 \tag{28}$$

- The 50 eigenvector with the largest eigenvalues of the matrix $\mathbf{B}$ from (20) are calculated (providing the spatial structure of the perturbation).

- From those 50 eigenvector/eigenvalues an ensemble of 51 members is created with zero mean (2nd order exact re-sampling).
- The GETM model is run for 40 days with each of those perturbed boundary values.
- Observations are assimilated with an expected RMS error of 0.3 m/s (including representativity error and error that cannot be corrected modifying only the boundary conditions) providing an optimal increment of the boundary values.
- The model is rerun with the optimized boundary values for 60 days.