

DIVA and DINEOF

Overview

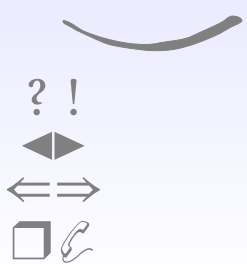
Jean-Marie Beckers and GHER group Aida Alvera, Alexander Barth, Charles Troupin, Mohamed Ouberdous, Sylvain Watelet, Igor Tomazic



<http://modb.oce.ulg.ac.be/GHER>

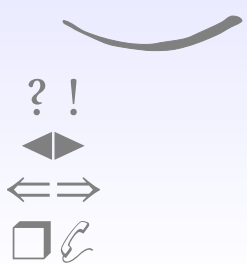


Université de Liège
MARE-GHER Sart-Tilman B5
4000 Liège, Belgique

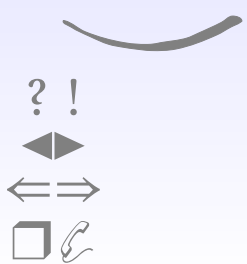


Outline

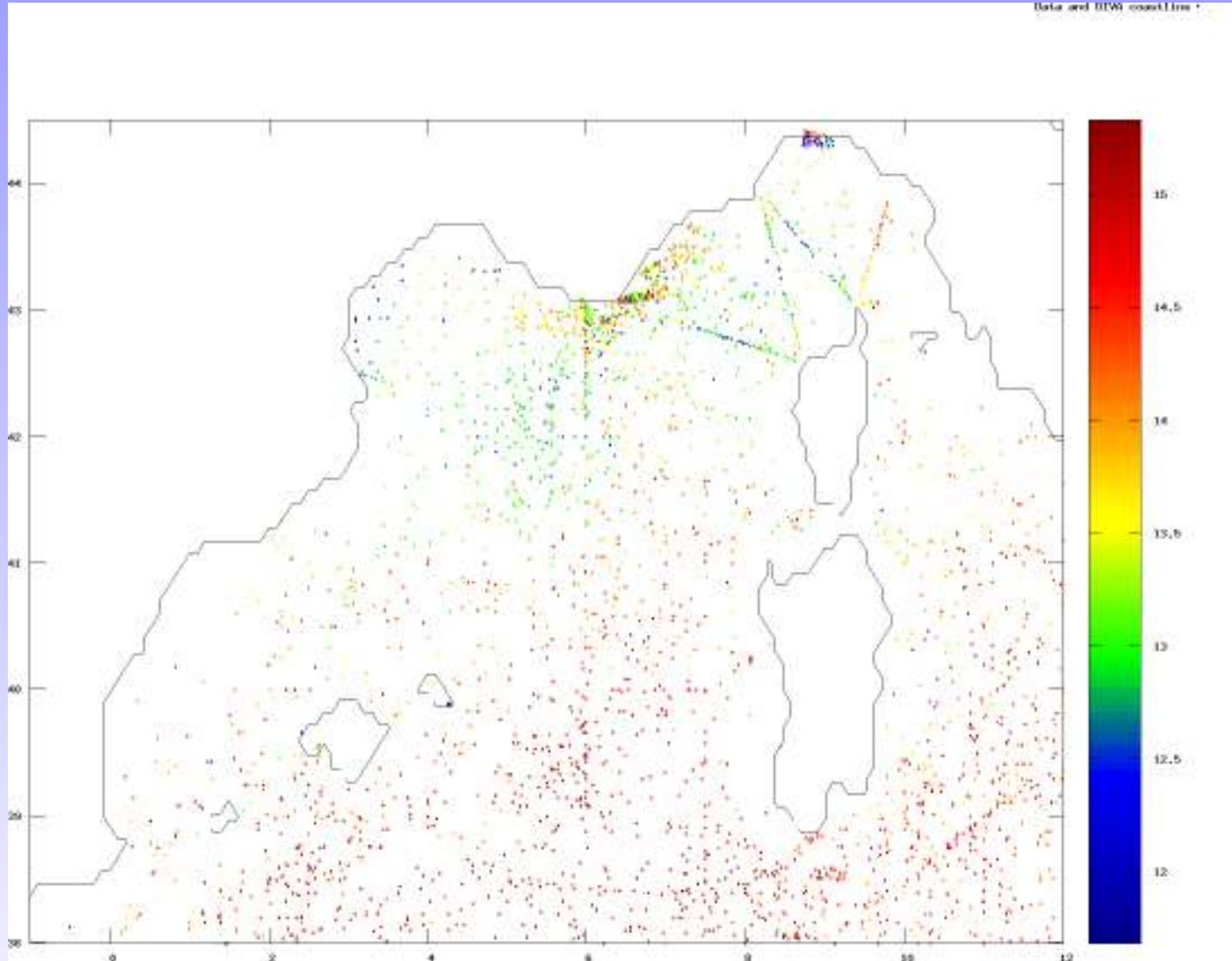
- ***Gridding***
- ***DIVA theory***
- ***Implementations and exercises***
- ***DINEOF theory***
- ***Implementations and exercises***



- **Gridding**
- *DIVA theory*
- *Implementations and exercises*
- *DINEOF theory*
- *Implementations and exercises*



Common problem

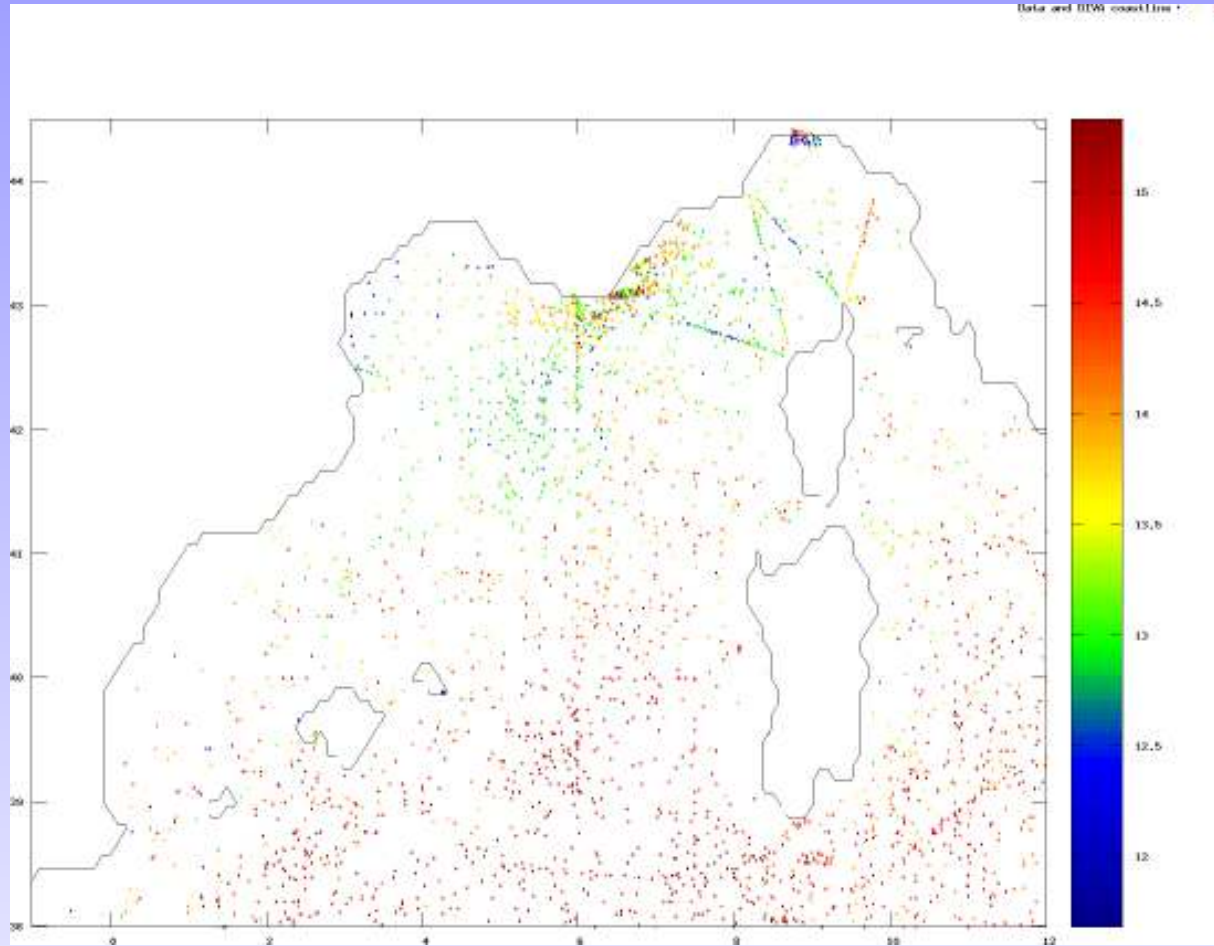


Appears when trying to produce maps, calculate volume averages, prepare initial conditions for models, quality control of data ...

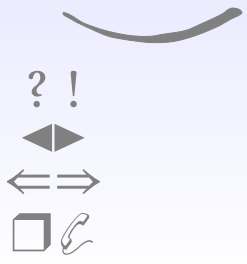
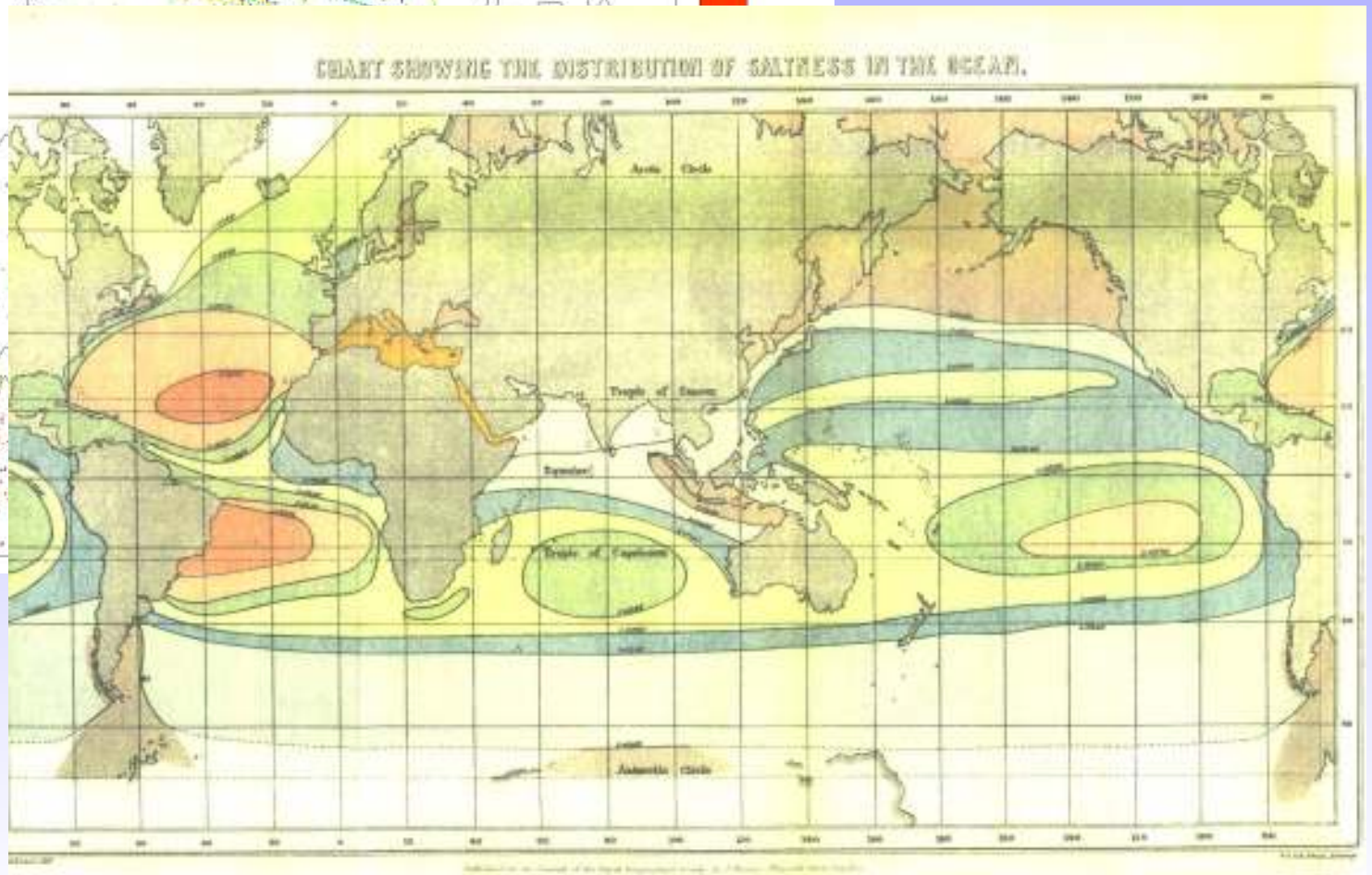
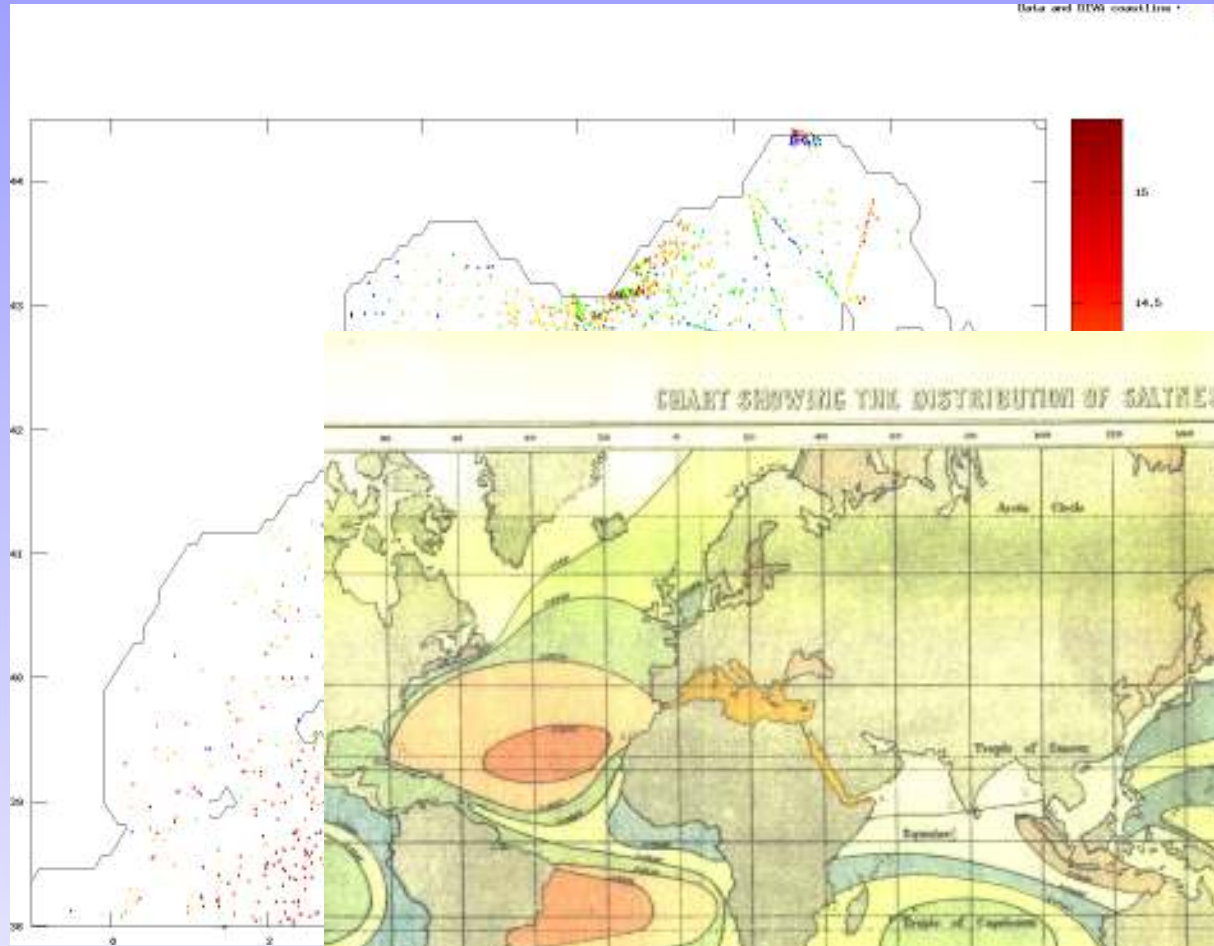
Université de Liège



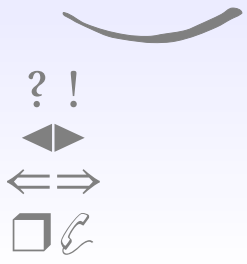
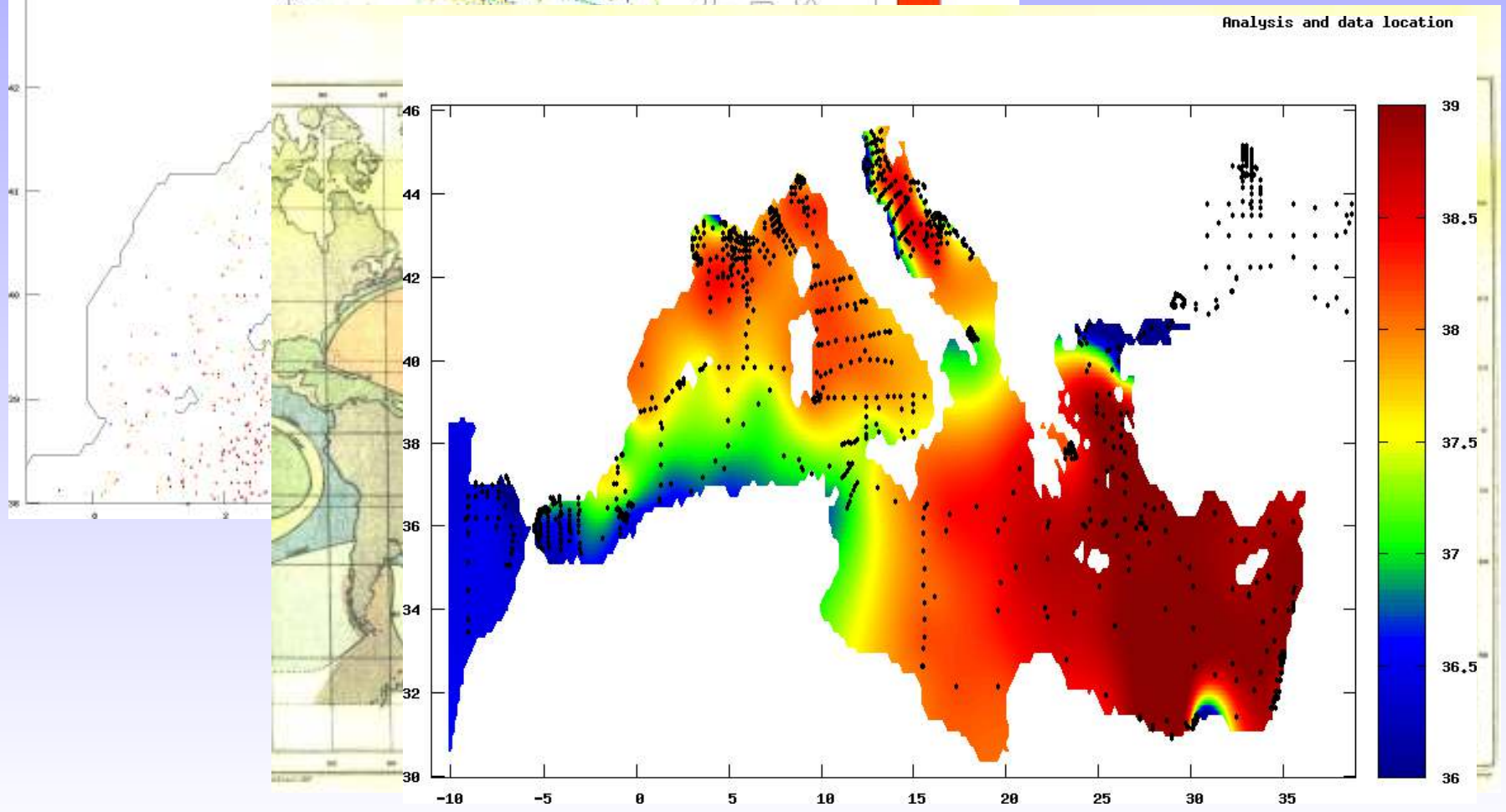
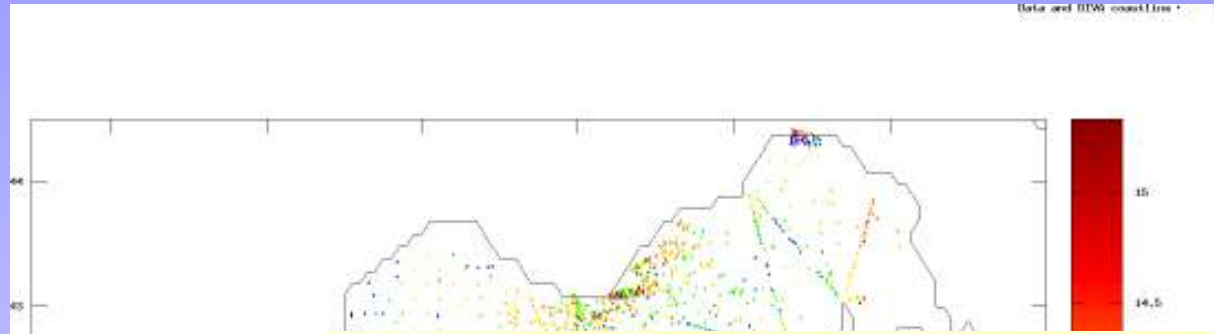
Solutions



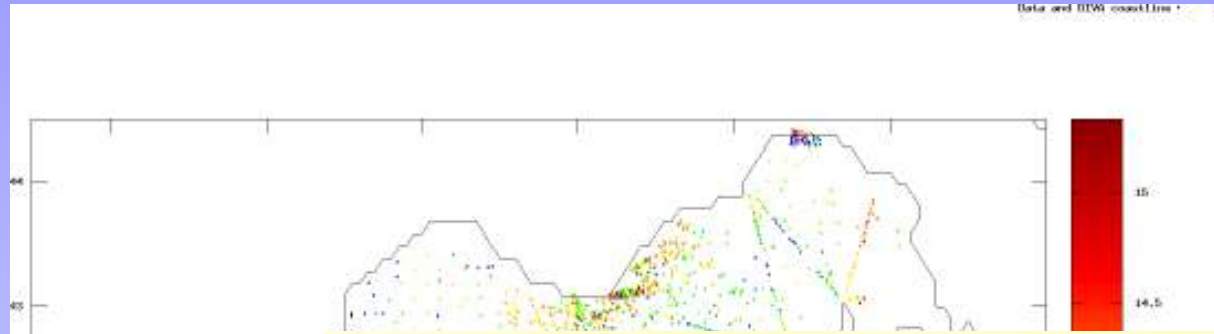
Solutions



Solutions



Solutions



MyOcean

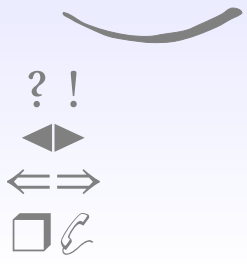
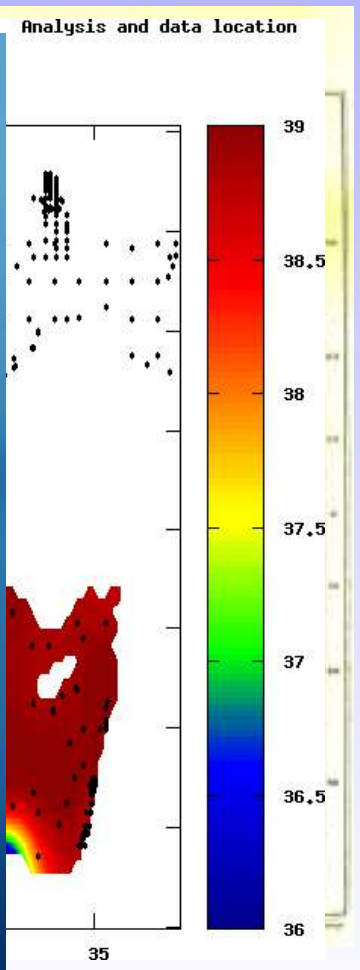
- Project
- Products & Services
- User's Feedback

Image of the month:
ARCTIC ICE ON THE MOVE

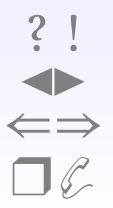
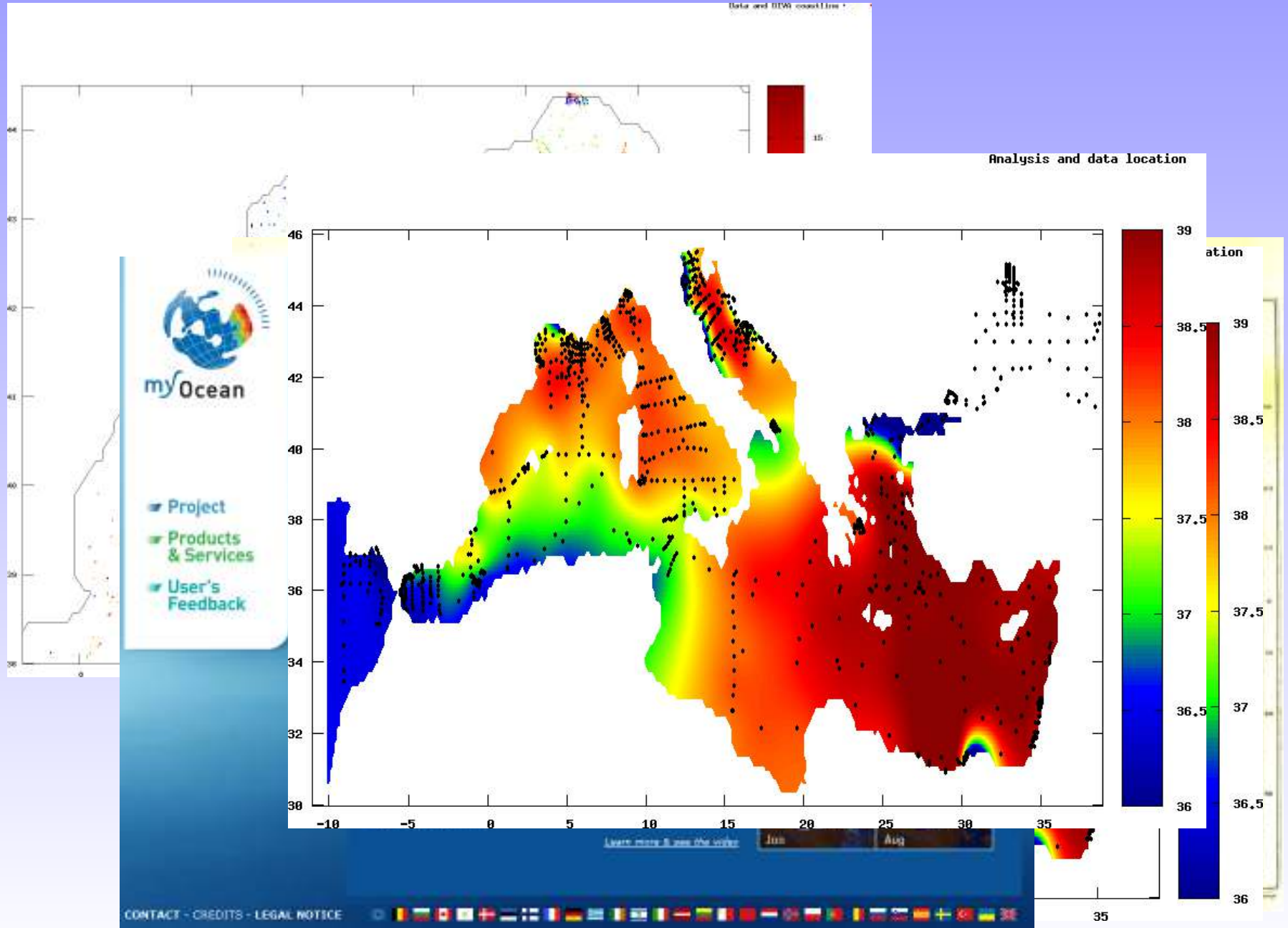
Ice extent record minima, the opening of the Northeast or Northwest Sea Passages. The Arctic is often in the news these days. Modelling and forecasting its moves as well as its reaction to climate change are important issues.

[Learn more & see the video](#)

CONTACT - CREDITS - LEGAL NOTICE



Solutions



Estimation of today's temperature in Delft

- Observer 1: 14°
- Observer 2: 16°

Your best guess ?

Estimation of today's temperature in Delft

- Observer 1: 14°
- Observer 2: 16°

Your best guess ?

15°

Estimation of today's temperature in Delft

- Observer 1: 14°
- Observer 2: 16°

Your best guess ?

But what if observer 1 uses digital thermometer and observer 2 his finger ?

Estimation of today's temperature in Delft

- Observer 1: 14°
- Observer 2: 16°

Your best guess ?

But what if observer 1 which uses digital thermometer is in Bruges and observer 2 which uses his his finger is in Delft ?

Estimation of today's temperature in Delft

- Observer 1: 14°
- Observer 2: 16°

Your best guess ?

But what if observer 1 which uses digital thermometer is in Sidney and observer 2 which uses his his finger is in Delft ?

Estimation of today's temperature in Delft

- Observer 1: 14°
- Observer 2: 16°

Your best guess ?

But what if observer 1 which uses digital thermometer is in Sidney and observer 2 which uses his his finger is in Delft ?

Best guess probably 16° but with a higher error bar

Exploit knowledge of errors and distance both for the estimate itself but also the error bars

Optimal interpolation

Exploit knowledge of errors and distance both for the estimate itself
but also the error bars

When done mathematically searching for the estimate with
lowest expected error: OPTIMAL INTERPOLATION

⚠ Optimal, but needs some statistical information

Optimal estimate of true state T^t

With two observations T_1 and T_2 deviation from the (unknown) truth T^t by (unknown) observational errors ϵ_1 and ϵ_2 :

$$T_1 = T^t + \epsilon_1, \quad \langle \epsilon_1 \rangle = 0, \quad T_2 = T^t + \epsilon_2, \quad \langle \epsilon_2 \rangle = 0 \quad (1)$$

statistical average, denoted by $\langle \quad \rangle$ with unbiased estimates $\langle \epsilon_* \rangle = 0$
 Linear estimate of the field

$$T = w_1 T_1 + w_2 T_2 = (w_1 + w_2) T^t + (w_1 \epsilon_1 + w_2 \epsilon_2) \quad (2)$$

$$\langle T \rangle = (w_1 + w_2) T^t, \quad (3)$$

we obtain an unbiased estimate of the true state if we take $w_1 + w_2 = 1$. This leaves one parameter free to chose: w_2

Exploit knowledge on errors to find optimal value of w_2

Choice of weighting ?

Analyzed field T^a calculated as

$$T^a = (1 - w_2)T_1 + w_2T_2 = T_1 + w_2(T_2 - T_1) \quad (4)$$

while in reality there is an error

$$T^a - T^t = (1 - w_2)\epsilon_1 + w_2\epsilon_2, \quad (5)$$

This error is zero on average but its variance is not zero:

$$\langle (T^a - T^t)^2 \rangle = (1 - w_2)^2 \langle \epsilon_1^2 \rangle + w_2^2 \langle \epsilon_2^2 \rangle + 2(1 - w_2)w_2 \langle \epsilon_1\epsilon_2 \rangle \quad (6)$$

The actual errors ϵ_1 and ϵ_2 are not known, but the error variance $\langle \epsilon_1^2 \rangle$ are. Often we can reasonably suppose that the errors ϵ_1 and ϵ_2 are uncorrelated $\langle \epsilon_1\epsilon_2 \rangle = 0$. The error variance $\langle \epsilon^2 \rangle$ of the analysis is then

$$\langle \epsilon^2 \rangle = (1 - w_2)^2 \langle \epsilon_1^2 \rangle + w_2^2 \langle \epsilon_2^2 \rangle. \quad (7)$$

So what ?

Minimisation

$$\langle \epsilon^2 \rangle = (1 - w_2)^2 \langle \epsilon_1^2 \rangle + w_2^2 \langle \epsilon_2^2 \rangle. \quad (8)$$

Naturally, the best estimate for T is the one with the lowest expected error variance and we will use w_2 , which minimizes the right-hand side:

$$w_2 = \frac{\langle \epsilon_1^2 \rangle}{\langle \epsilon_1^2 \rangle + \langle \epsilon_2^2 \rangle} \quad (9)$$

$$T^a = \frac{\langle \epsilon_1^2 \rangle \langle \epsilon_2^2 \rangle}{\langle \epsilon_1^2 \rangle + \langle \epsilon_2^2 \rangle} \left(\frac{T_1}{\langle \epsilon_1^2 \rangle} + \frac{T_2}{\langle \epsilon_2^2 \rangle} \right). \quad (10)$$

Best estimate

With (9) we obtain the minimal error variance

$$\langle \epsilon^2 \rangle = \frac{\langle \epsilon_1^2 \rangle \langle \epsilon_2^2 \rangle}{\langle \epsilon_1^2 \rangle + \langle \epsilon_2^2 \rangle} = \left(1 - \frac{\langle \epsilon_1^2 \rangle}{\langle \epsilon_1^2 \rangle + \langle \epsilon_2^2 \rangle} \right) \langle \epsilon_1^2 \rangle, \quad (11)$$

while the estimate of the temperature itself reads also

$$T^a = T_1 + \left(\frac{\langle \epsilon_1^2 \rangle}{\langle \epsilon_1^2 \rangle + \langle \epsilon_2^2 \rangle} \right) (T_2 - T_1). \quad (12)$$

Error variance on the combination of T_1 and T_2 is smaller than both $\langle \epsilon_1^2 \rangle$ and $\langle \epsilon_2^2 \rangle$.

VAR approach

Same solution by

$$\min_T J = \frac{(T - T_1)^2}{2\langle \epsilon_1^2 \rangle} + \frac{(T - T_2)^2}{2\langle \epsilon_2^2 \rangle}. \quad (13)$$

Optimal interpolation

Analysis x^a as a linear combination of the forecast x^f and the observations y :

$$x^a = x^f + \mathbf{K} (y - \mathbf{H}x^f) \quad (14)$$

\mathbf{H} observation operator and innovation vector

$$d = y - \mathbf{H}x^f \quad (15)$$

Objective: prescribe an optimal matrix \mathbf{K} : Kalman gain matrix

Knowledge on error distribution

$$\boldsymbol{\epsilon} = \mathbf{x} - \mathbf{x}^t \quad (16)$$

$$\boldsymbol{\epsilon}^o = \mathbf{y} - \mathbf{y}^t. \quad (17)$$

Error-covariance matrix

$$\mathbf{R} = \langle \boldsymbol{\epsilon}^o \boldsymbol{\epsilon}^{oT} \rangle \quad (18)$$

is semi-positive defined since $\mathbf{z}^T \mathbf{R} \mathbf{z} = \langle (\mathbf{z}^T \boldsymbol{\epsilon}^o)^2 \rangle$

The analysis step (14) reads

$$\mathbf{x}^t + \boldsymbol{\epsilon}^a = \mathbf{x}^t + \boldsymbol{\epsilon}^f + \mathbf{K} \left(\boldsymbol{\epsilon}^o - \mathbf{H} \boldsymbol{\epsilon}^f \right) + \underbrace{\mathbf{K} \left(\mathbf{y}^t - \mathbf{H} \mathbf{x}^t \right)}_{=0} \quad (19)$$

Kalman gain

$$\boldsymbol{\epsilon}^a = \boldsymbol{\epsilon}^f + \mathbf{K} (\boldsymbol{\epsilon}^o - \mathbf{H}\boldsymbol{\epsilon}^f). \quad (20)$$

Construct the error covariance $\langle \boldsymbol{\epsilon}^a \boldsymbol{\epsilon}^{aT} \rangle$ of the analysis by multiplying (20) by its transposed and take the statistical average or expectation

$$\begin{aligned} \langle \boldsymbol{\epsilon}^a \boldsymbol{\epsilon}^{aT} \rangle &= \langle \boldsymbol{\epsilon}^f \boldsymbol{\epsilon}^{fT} \rangle + \mathbf{K} \langle (\boldsymbol{\epsilon}^o - \mathbf{H}\boldsymbol{\epsilon}^f) \boldsymbol{\epsilon}^{fT} \rangle + \langle \boldsymbol{\epsilon}^f (\boldsymbol{\epsilon}^{oT} - \boldsymbol{\epsilon}^{fT} \mathbf{H}^T) \rangle \mathbf{K}^T \\ &+ \mathbf{K} \langle (\boldsymbol{\epsilon}^o - \mathbf{H}\boldsymbol{\epsilon}^f) (\boldsymbol{\epsilon}^{oT} - \boldsymbol{\epsilon}^{fT} \mathbf{H}^T) \rangle \mathbf{K}^T. \end{aligned} \quad (21)$$

Define covariance matrices

$$\mathbf{P} = \langle \boldsymbol{\epsilon} \boldsymbol{\epsilon}^T \rangle \quad (22)$$

and assume that observational errors and model errors are not correlated, $\langle \boldsymbol{\epsilon}^o \boldsymbol{\epsilon}^T \rangle = 0$.

Kalman gain

The error-covariance matrix after analysis can then be written as

$$\begin{aligned} \mathbf{P}^a &= \mathbf{P}^f - \mathbf{KHP}^f - \mathbf{P}^f \mathbf{H}^T \mathbf{K}^T + \mathbf{K} \left(\mathbf{R} + \mathbf{HP}^f \mathbf{H}^T \right) \mathbf{K}^T \\ &= \mathbf{P}^f - \mathbf{P}^f \mathbf{H}^T \mathbf{A}^{-1} \mathbf{HP}^f + \left(\mathbf{P}^f \mathbf{H}^T - \mathbf{KA} \right) \mathbf{A}^{-1} \left(\mathbf{HP}^f - \mathbf{AK}^T \right) \end{aligned} \quad (23)$$

where we define matrix

$$\mathbf{A} = \mathbf{HP}^f \mathbf{H}^T + \mathbf{R} \quad (24)$$

which is symmetric and we suppose that it can be inverted. Global error estimate:

$$\epsilon^a = \left\langle \boldsymbol{\epsilon}^{aT} \boldsymbol{\epsilon}^a \right\rangle = \text{trace } \mathbf{P}^a. \quad (25)$$

Search for an optimal \mathbf{K} which minimizes this trace or for which

$$\epsilon^a(\mathbf{K} + \mathbf{L}) - \epsilon^a(\mathbf{K}) = 0 \quad (26)$$

for any small departure matrix \mathbf{L}

Kalman gain

$$\text{trace} -\mathbf{L} \left(\mathbf{H} \mathbf{P}^f - \mathbf{A} \mathbf{K}^T \right) - \left(\mathbf{P}^f \mathbf{H}^T - \mathbf{K} \mathbf{A} \right) \mathbf{L}^T = 0, \quad (27)$$

where we neglected quadratic terms in \mathbf{L} . The two terms are the transposed version of each other and since the trace of the matrix and its transposed are identical, we must request

$$\text{trace} \left(\mathbf{P}^f \mathbf{H}^T - \mathbf{K} \mathbf{A} \right) \mathbf{L}^T = 0.$$

Since \mathbf{L} is arbitrary, the optimal solution with minimum error is obtained when

$$\mathbf{K} = \mathbf{P}^f \mathbf{H}^T \mathbf{A}^{-1} = \mathbf{P}^f \mathbf{H}^T \left(\mathbf{H} \mathbf{P}^f \mathbf{H}^T + \mathbf{R} \right)^{-1} \quad (28)$$

Kalman gain

The error covariance of the analysis is obtained by injecting (28) into (23)

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H}) \mathbf{P}^f = \left(\mathbf{I} - \mathbf{P}^f \mathbf{H}^T (\mathbf{H} \mathbf{P}^f \mathbf{H}^T + \mathbf{R})^{-1} \mathbf{H} \right) \mathbf{P}^f \quad (29)$$

which is the analogue of (11). Note that both the Kalman gain matrix and the error covariance after the analysis do not depend on the *value* of the observations or the forecasted state vector but only on their statistical error covariances. The only field that depends on the actual values is of course the state vector itself:

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{P}^f \mathbf{H}^T (\mathbf{H} \mathbf{P}^f \mathbf{H}^T + \mathbf{R})^{-1} (\mathbf{y} - \mathbf{H} \mathbf{x}^f). \quad (30)$$

The use of (28) in (14) to combine the forecast and observation with prescribed error covariance \mathbf{P}^f and \mathbf{R} is known as optimal interpolation (OI)

3D-Var

Find the state vector that minimizes the error measure J given by

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^f)^T \mathbf{P}^f{}^{-1}(\mathbf{x} - \mathbf{x}^f) + \frac{1}{2}(\mathbf{H}\mathbf{x} - \mathbf{y})^T \mathbf{R}^{-1}(\mathbf{H}\mathbf{x} - \mathbf{y}) \quad (31)$$

Yields the same optimal state.

3D-Var

Find the state vector that minimizes the error measure J given by

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^f)^T \mathbf{P}^f (\mathbf{x} - \mathbf{x}^f) + \frac{1}{2}(\mathbf{H}\mathbf{x} - \mathbf{y})^T \mathbf{R}^{-1}(\mathbf{H}\mathbf{x} - \mathbf{y}) \quad (32)$$

Yields the same optimal state.

VAR minimizes a sum of a quadratic term of the state-variables and a quadratic term of misfits (residuals)

3D-Var

Find the state vector that minimizes the error measure J given by

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^f)^T \mathbf{P}^f{}^{-1}(\mathbf{x} - \mathbf{x}^f) + \frac{1}{2}(\mathbf{H}\mathbf{x} - \mathbf{y})^T \mathbf{R}^{-1}(\mathbf{H}\mathbf{x} - \mathbf{y}) \quad (33)$$

Yields the same optimal state.

VAR minimizes a sum of a quadratic term of the state-variables and a quadratic term of misfits (residuals)

Kalman filter and 3DVAR yield same results when used with same covariances in linear case.

Spatial interpolation

- "Model forecast": Background field (data mean, global spatial south-north gradient, climatological mean, ...)
- $\mathbf{B} = \mathbf{H}\mathbf{P}^f\mathbf{H}^T$: covariance of the background field between data points: element i, j of \mathbf{B} is the covariance between points in location i and j . Covariance between a given point and all data points is stored in column vector \mathbf{c} with local variance σ^2 .
- Analysis ϕ of anomaly \mathbf{y} with respect to background leads to spatial analysis at any desired location of covariance between any two points is known.

$$\phi = \mathbf{c}^T (\mathbf{B} + \mathbf{R})^{-1} \mathbf{y} \quad (34)$$

with a local error variance of the analysis

$$\epsilon_a^2 = \sigma^2 - \mathbf{c}^T (\mathbf{B} + \mathbf{R})^{-1} \mathbf{c} \quad (35)$$

⚠ Note that inversion of matrix is needed (cost \propto cube of number of data points).

Background covariance

Problem, how to specify background covariances (between all data points and between data points and the desired analysis location).

- c_i = covariance between location of the analysis and data location of point $i = C(x, x_i)$
- B_{ij} = covariance between location of data point i and location of point $j = C(x_i, x_j)$

Approaches

- Normally obtained via statistics on data. Seldom possible (noticable exception: satellite images, see DINEOF).
- Standard OI: via functions $B_{ij} = f(r/L)$ where r is the distance between points i and j , but still function f needs to be determined. L is the so-called correlation length. Here statistics on all data couples as a function of distance. Example: $f = \sigma^2 \exp(-r^2/L^2)$.
- Via functionals (see [Kernel](#) of DIVA later)

Signal to noise ratio

$$\mathbf{B} = \sigma^2 \tilde{\mathbf{B}} \quad (36)$$

$$\mathbf{R} = \epsilon^2 \tilde{\mathbf{R}} \quad (37)$$

$$\mathbf{c} = \sigma^2 \tilde{\mathbf{c}} \quad (38)$$

with non-dimensional correlation matrices $\tilde{\mathbf{B}}$, $\tilde{\mathbf{R}}$, $\tilde{\mathbf{c}}$

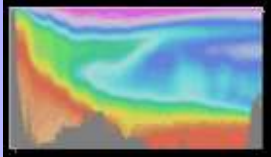
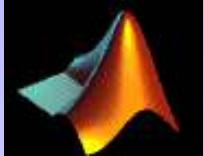


$$\phi = \tilde{\mathbf{c}}^T \left(\tilde{\mathbf{B}} + \frac{1}{\lambda} \tilde{\mathbf{R}} \right)^{-1} \mathbf{y} \quad (39)$$

with signal-to noise ratio

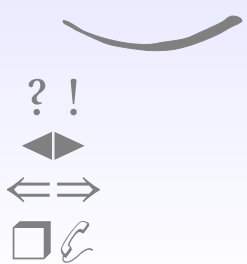
$$\lambda = \frac{\sigma^2}{\epsilon^2} \quad (40)$$

Also the error field is only depending on the ratio.

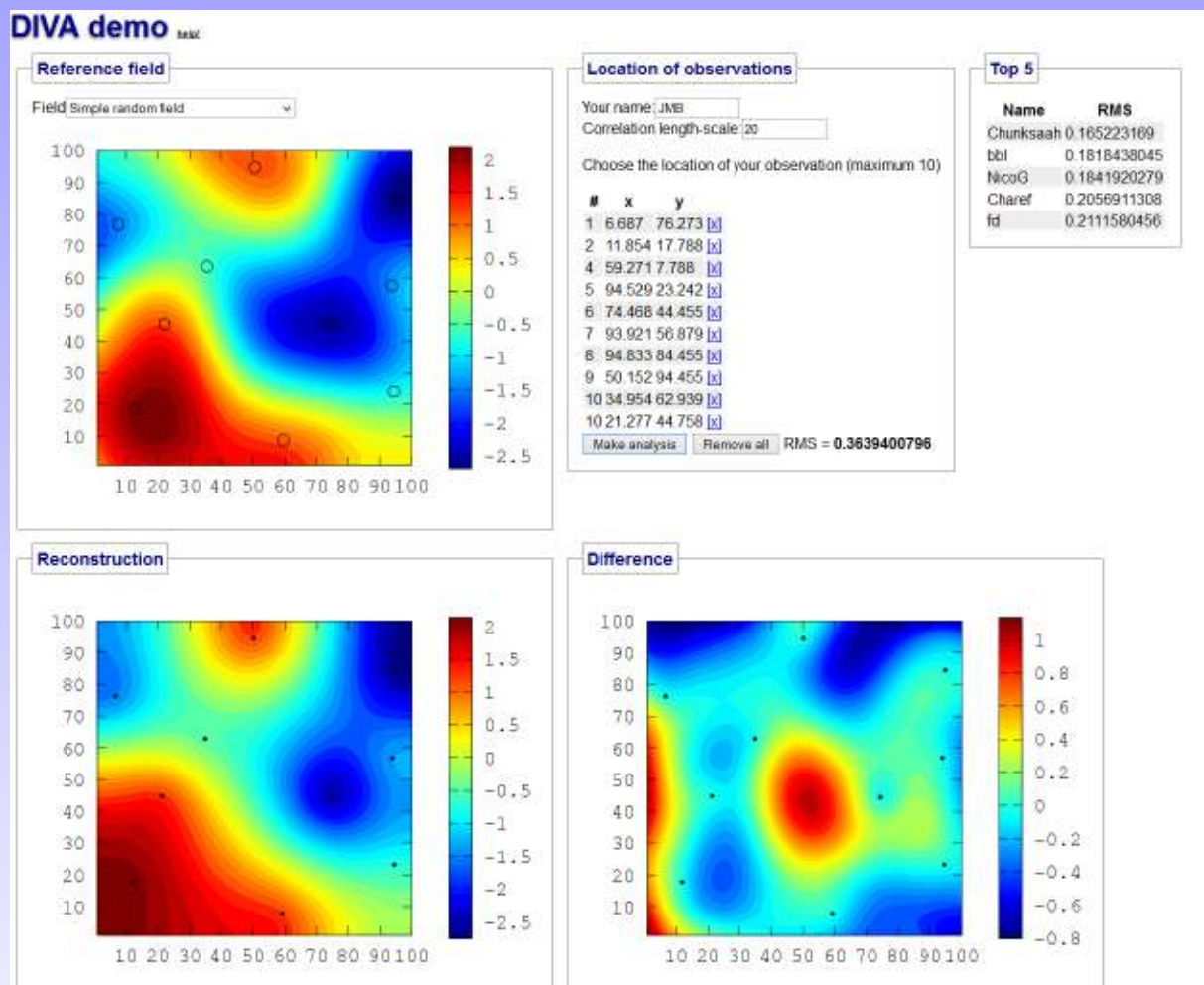
Statistical spatial analysis

Tools	Formats	Method
	ODV spreadsheet WOCE WOA ...	Dist. weighting, VIM
	netCDF (toolbox), CSV ascii, ...	Polynomial interpolation ...
	CSV ascii, ...	Kriging, OI, ...
	ODV spreadsheet	Variational

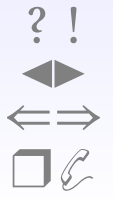
Mostly graphics oriented, without "oceanographic" knowledge.



Demo tool to feel effect of L



http://www.data-assimilation.net/Tools/divand_demo/html/



- *Gridding*
- ***DIVA theory***
- *Implementations and exercises*
- *DINEOF theory*
- *Implementations and exercises*

DIVA Basics

Variational Inverse Method, (Brasseur *et al.*, 1996). Knowing data d_j at location (x_j, y_j) , search the field φ which minimizes

$$J[\varphi] = \sum_{j=1}^{Nd} \mu_j [d_j - \varphi(x_j, y_j)]^2 + \|\varphi - \varphi_b\|^2 \quad (41)$$

$$\|\varphi\| = \int_D (\alpha_2 \nabla \nabla \varphi : \nabla \nabla \varphi + \alpha_1 \nabla \varphi \cdot \nabla \varphi + \alpha_0 \varphi^2) dD \quad (42)$$

The background field φ_b is typically the data average value.

- α_0 penalizes the field itself (anomalies),
- α_1 penalizes gradients $\nabla \varphi$ (no spatial trends),
- α_2 penalizes variability (regularization of second derivatives $\nabla \nabla \varphi$),
- α_* can be related to a length scale L of the analysis,
- μ_j penalizes data-analysis misfits (objective).

Basics

$$\mu = \frac{\sigma^2}{\epsilon^2} \frac{4\pi}{L^2} \quad (43)$$

where the σ^2/ϵ^2 is known as a signal to noise ratio S/N .



Solution by finite element method. Note decoupling of sub-basins.
(Each element is in fact composed by three sub-elements, each one with cubic functions)



Bad news ☹️

- No error estimate comes with the method, only an indicator of data-coverage.

Bad news ☹

- No error estimate comes with the method, only an indicator of data-coverage.



- VIM brand already taken:



Bad news ☹

- No error estimate comes with the method, only an indicator of data-coverage.



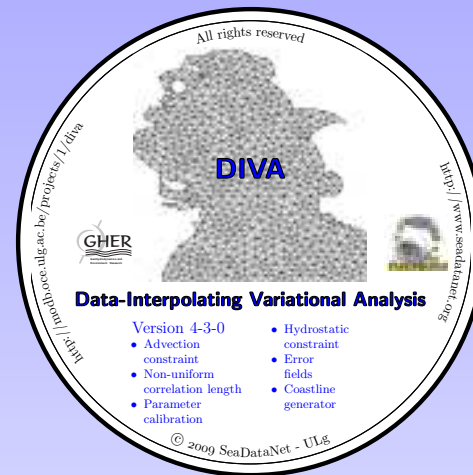
- VIM brand already taken:



- Method is equivalent to well established existing optimal interpolation (OI)

Good news 😊

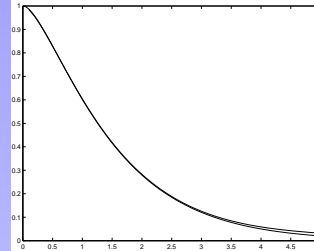
- Name easily changed: DIVA (Data-Interpolating Variational Analysis)



- Optimal interpolation (OI) provides error estimates, so DIVA can also provide it via equivalence
- DIVA has some practical advantages over OI

DIVA as OI

DIVA is identical to the well known Optimal Interpolation



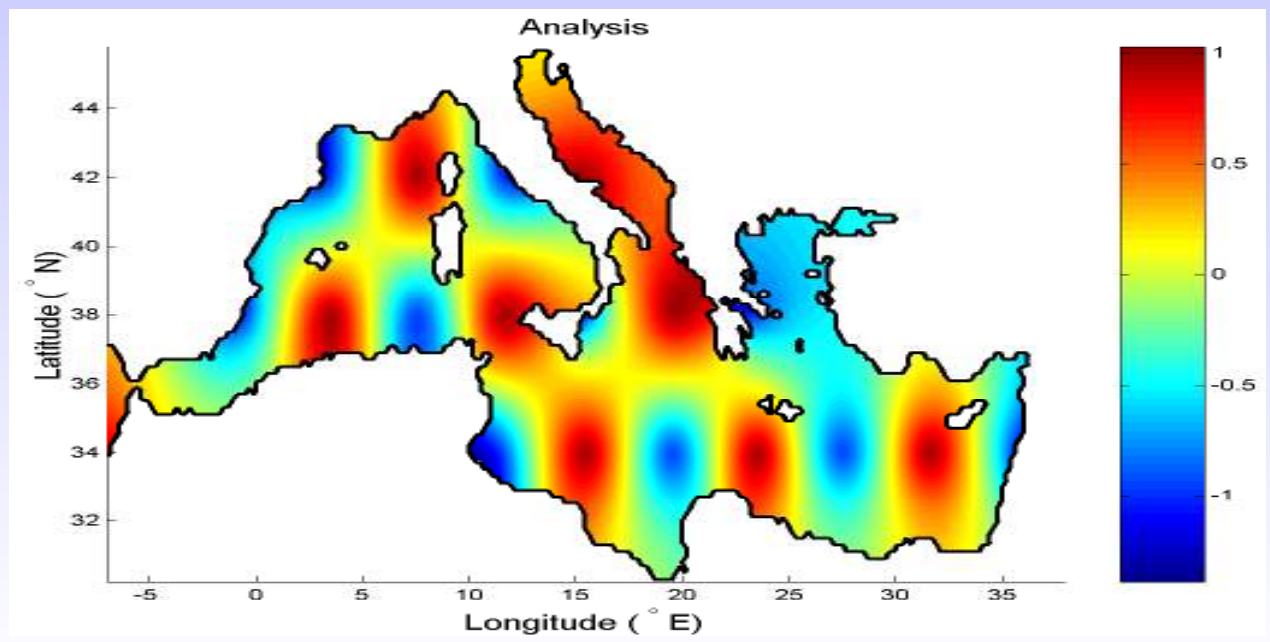
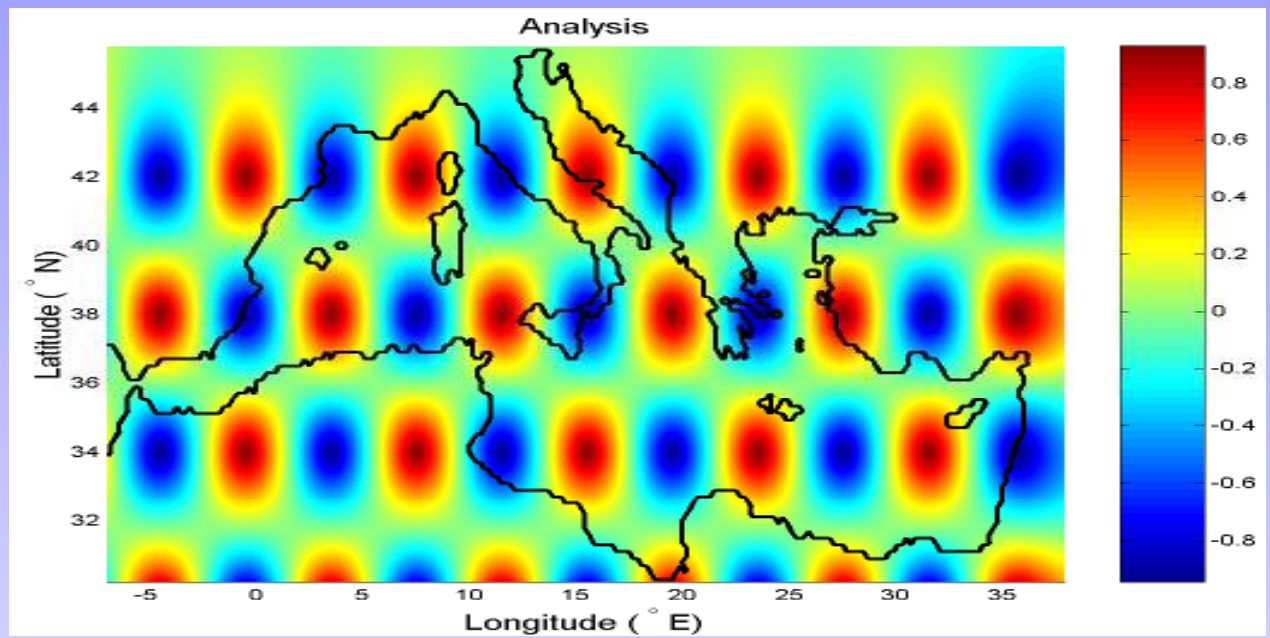
- if so-called reproducing kernel of the norm = [covariance function](#) of OI,
- if the noise is random, spatially uncorrelated and the signal/noise ratio parameter is identical with OI.

In this case, the OI solution = DIVA solution.

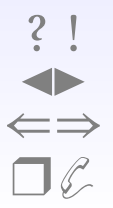
- Advantages of DIVA: regularization, fast finite-element solution, boundary effects taken into account.
- Difficulties: generalizations to 3D and multivariate versions are "hybrid".

Major direct advantage of DIVA: matrix to invert is related to the finite-element mesh, NOT the number of data. Useful for large data sets (Rixen *et al.*, 2000). Equivalence allows to calculate error fields with DIVA even if formulation does not rely on error minimization.

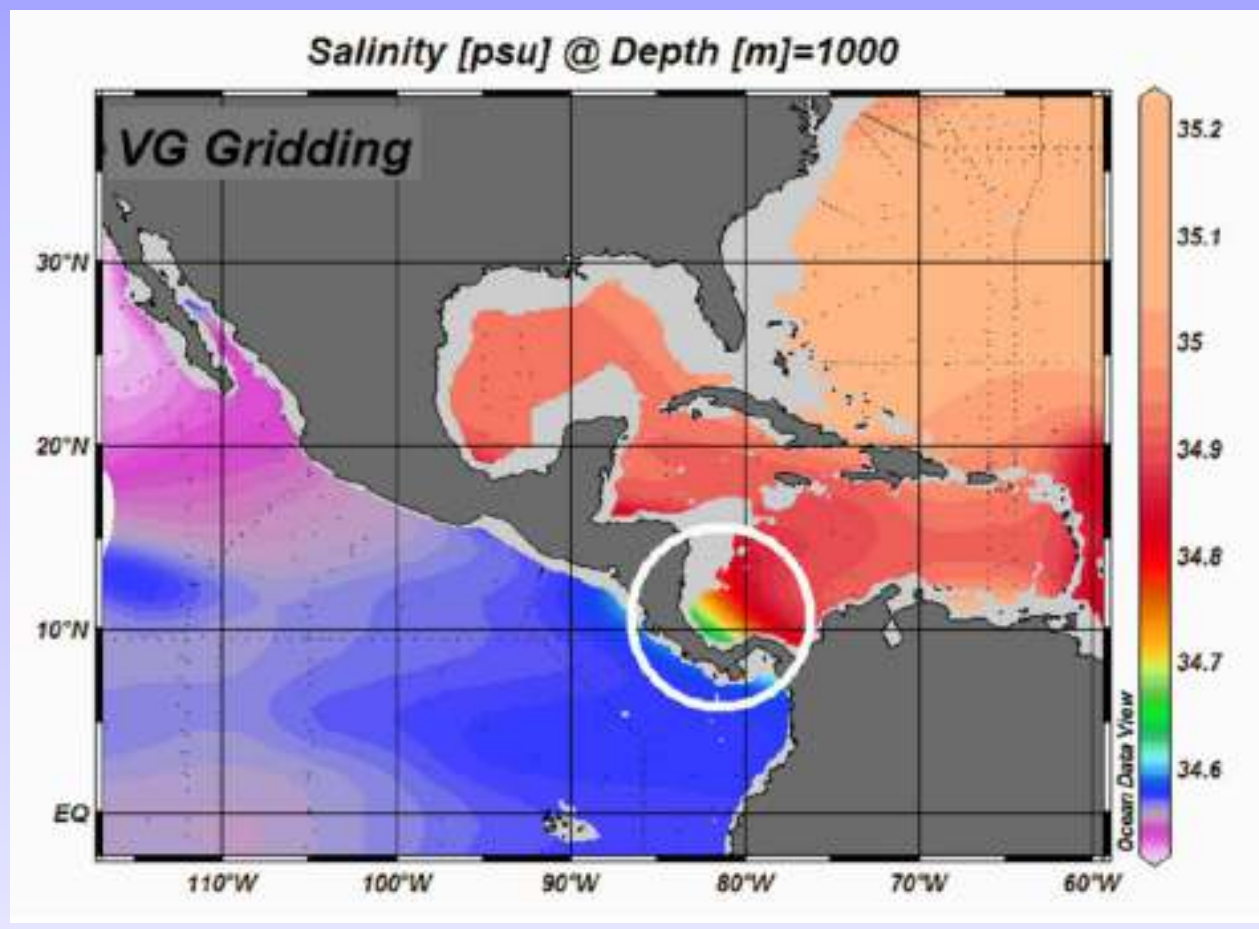
Illustration of covariance functions



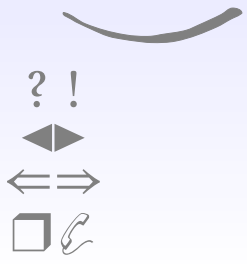
Université de Liège



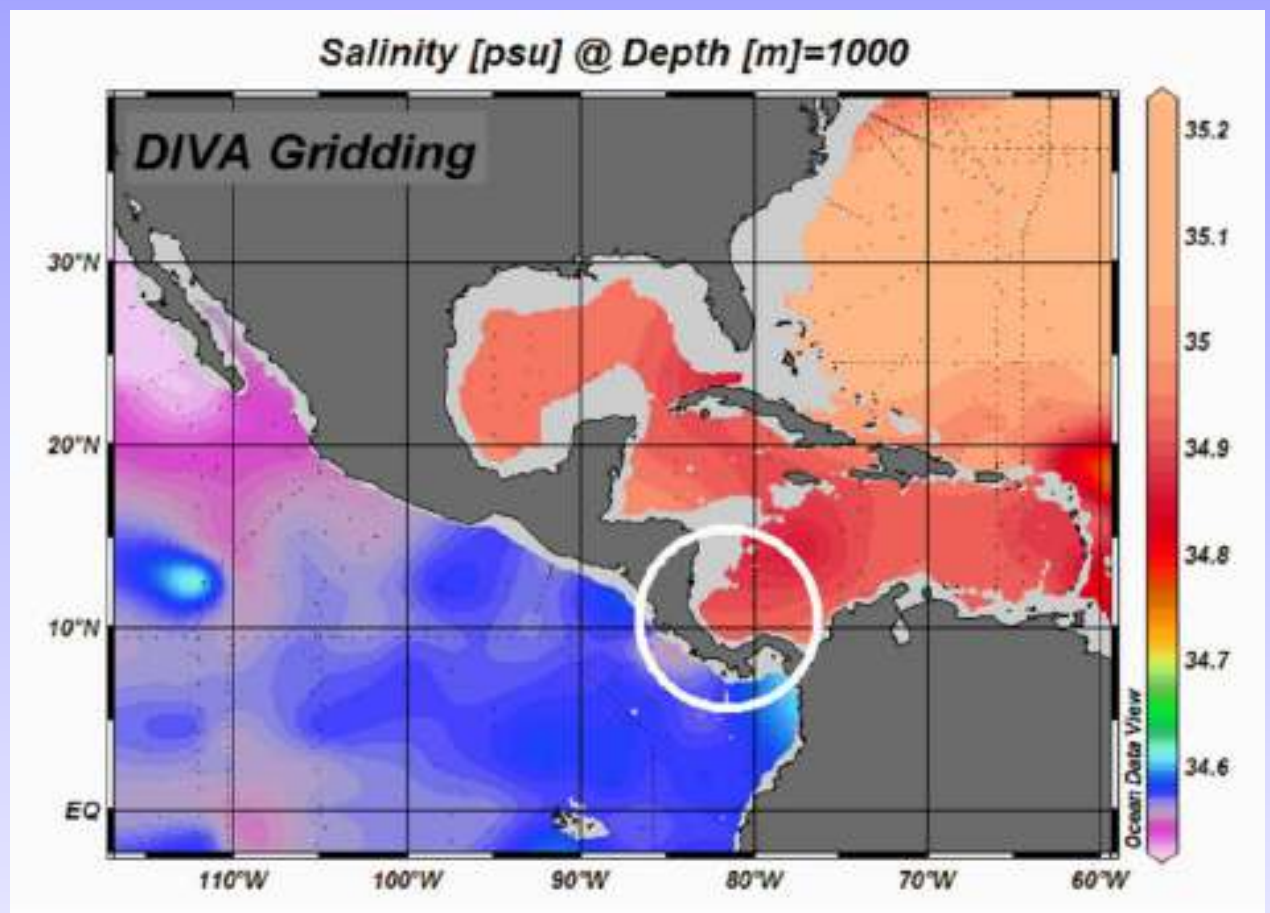
Standard ODV analysis



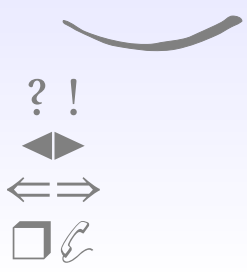
(R. Schlitzer ODV example)



ODV-DIVA analysis



(R. Schlitzer ODV example)



Additions to basic tool

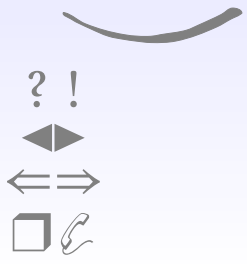
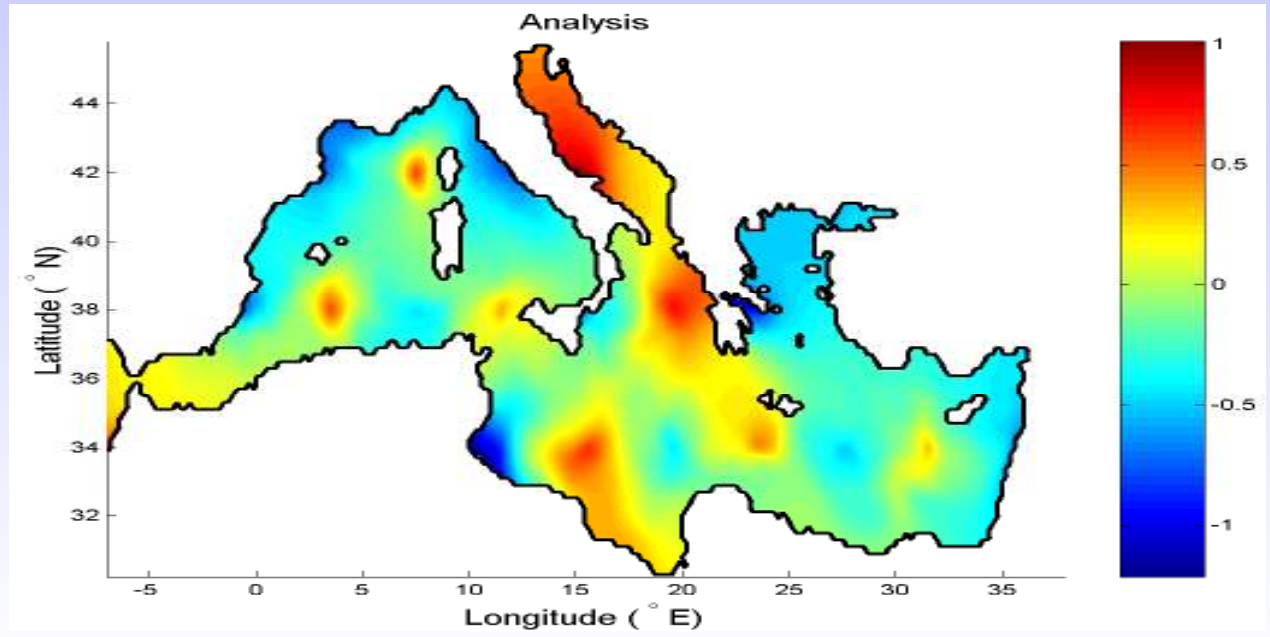
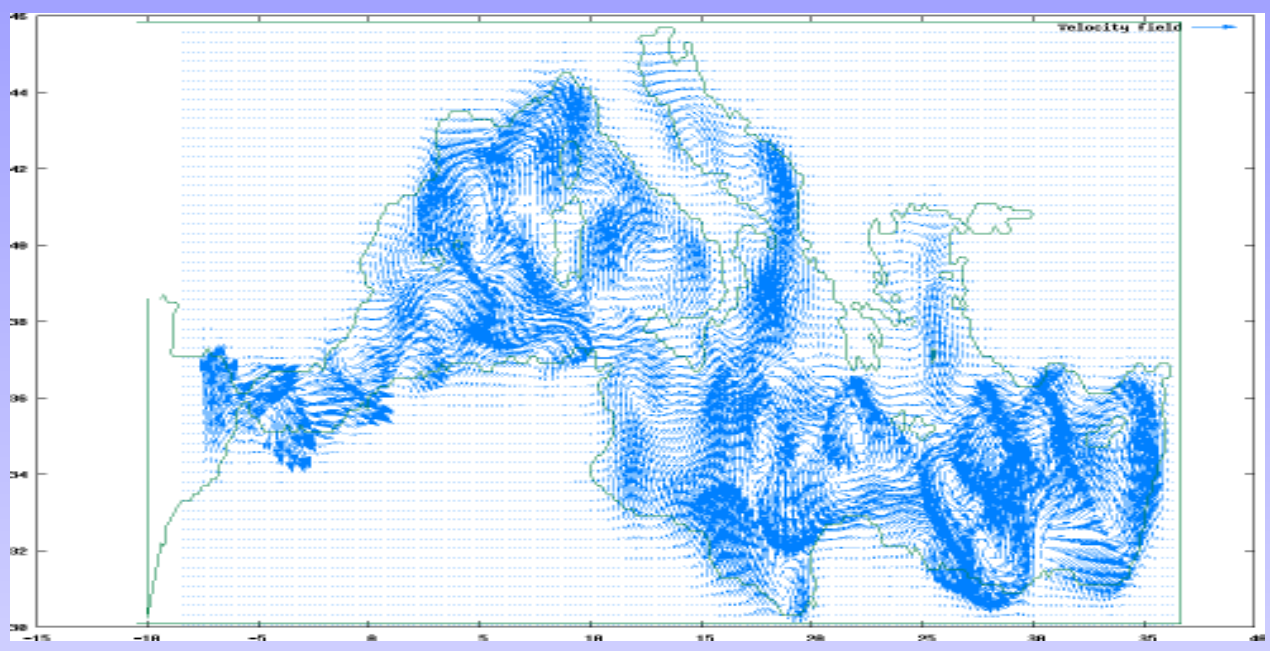
Advection constraint: Augmented cost function to deal with preferred correlation directions, eg, via advection with velocity \mathbf{u} and diffusion \mathcal{A}

$$J_a = J(\varphi) + \theta \int_D [\mathbf{u} \cdot \nabla \varphi - \mathcal{A} \nabla \cdot \nabla \varphi]^2 dD \quad (44)$$

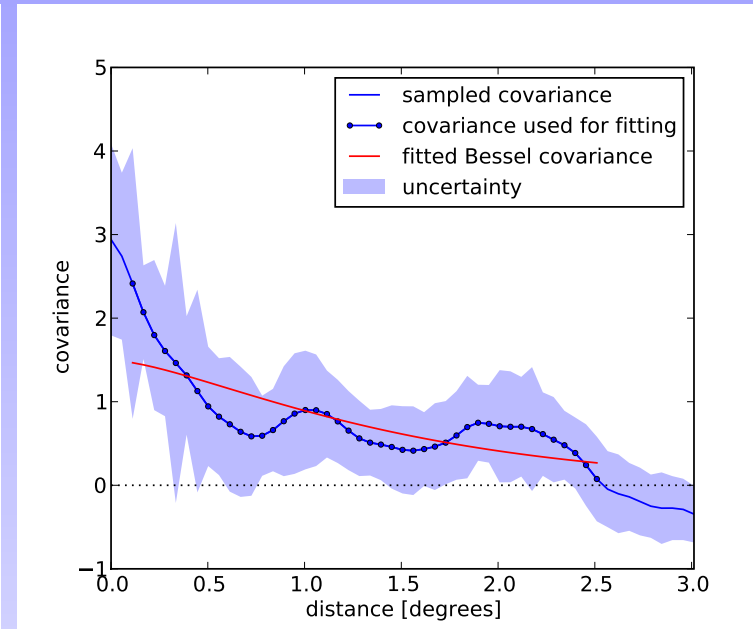
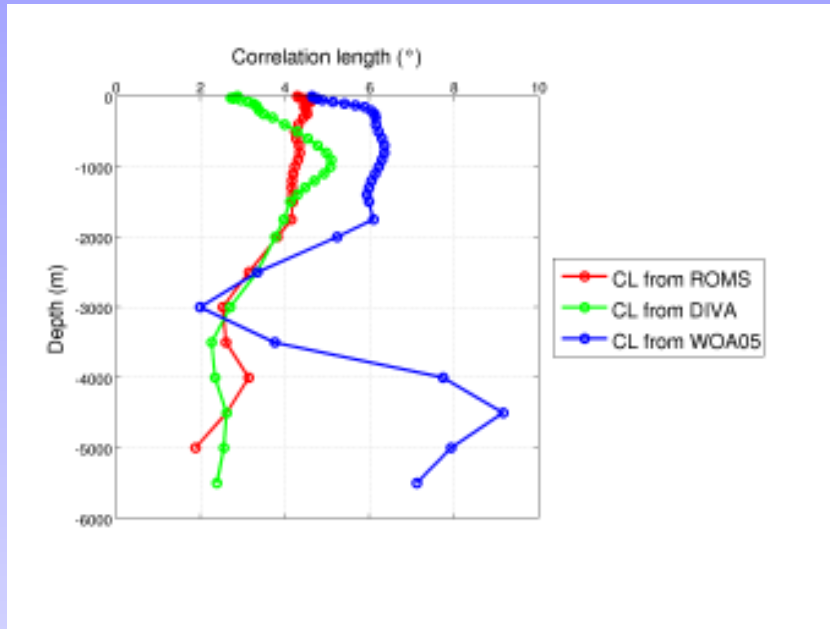
Other features

- Error fields taking data distribution into account.
- Toolbox approach allowing to design own versions.
- 3D and 4D modes by looping, hydrostatic constraint in 3D mode.
- Cross validation tools to infer statistical parameters and error estimates.
- Climatology production version with heterogeneous data distributions [\(detrending\)](#).
- Outlier detection.
- Variable correlation length.
- ...

Covariances with advection



Parameter calibration

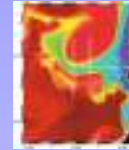


Spatial coherence of parameters: here correlation length obtained with covariance fitting (Troupin *et al.*, 2010).



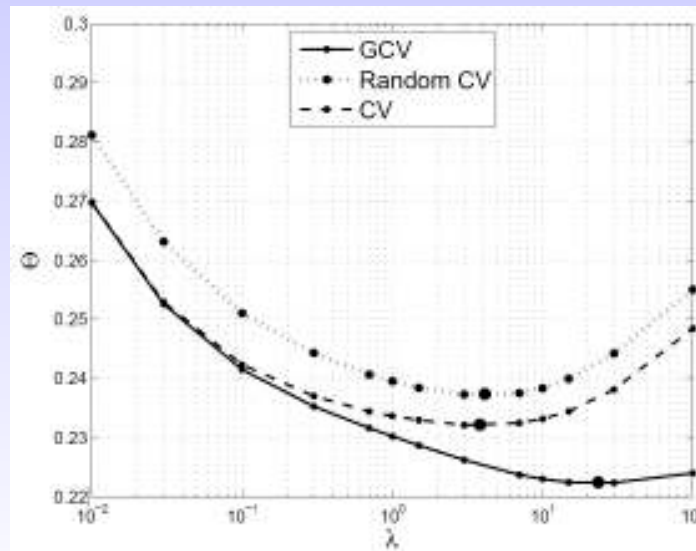
Signal to noise ratio

The most elusive parameter.



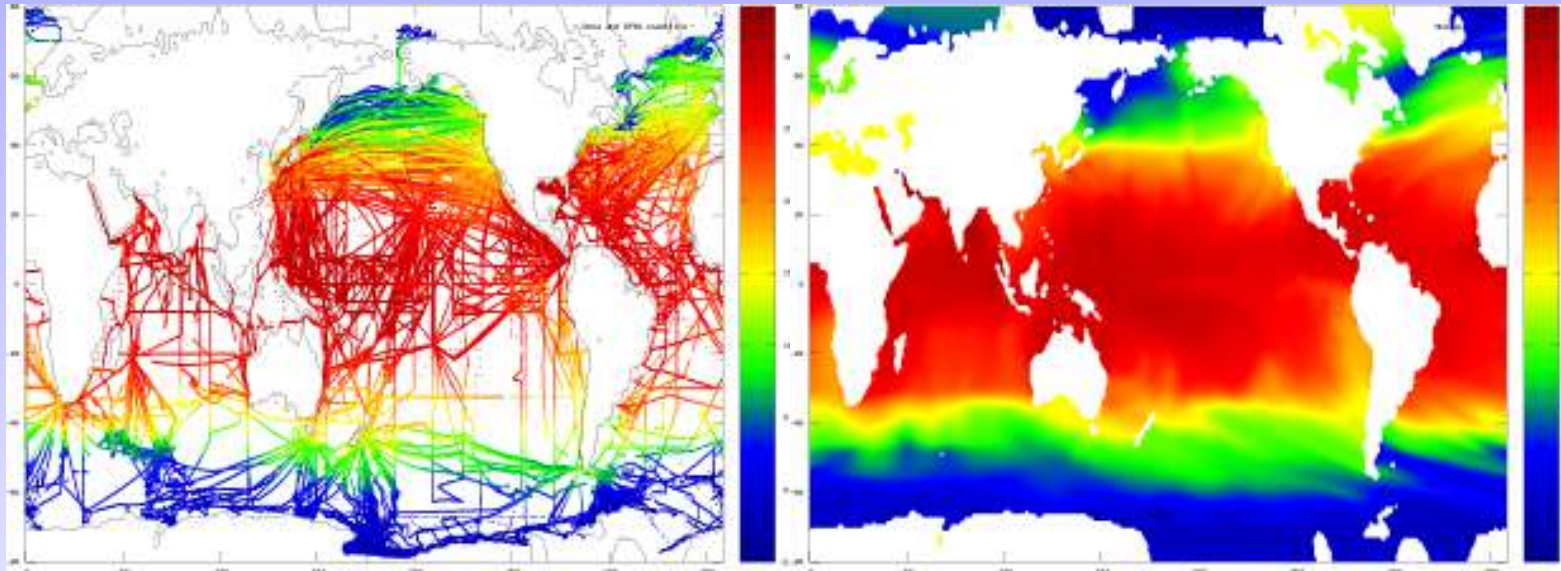
- Noise is not only instrumental error:
- Very hard problem to decide on value with dependent data (cross-validation approaches fail).

A series of estimation tools are provided with DIVA, but here the experience of oceanographers is critical. A posteriori analysis of residuals allows to verify coherence. With reasonable amount of data, parameter not critical for analysis but for error estimates.

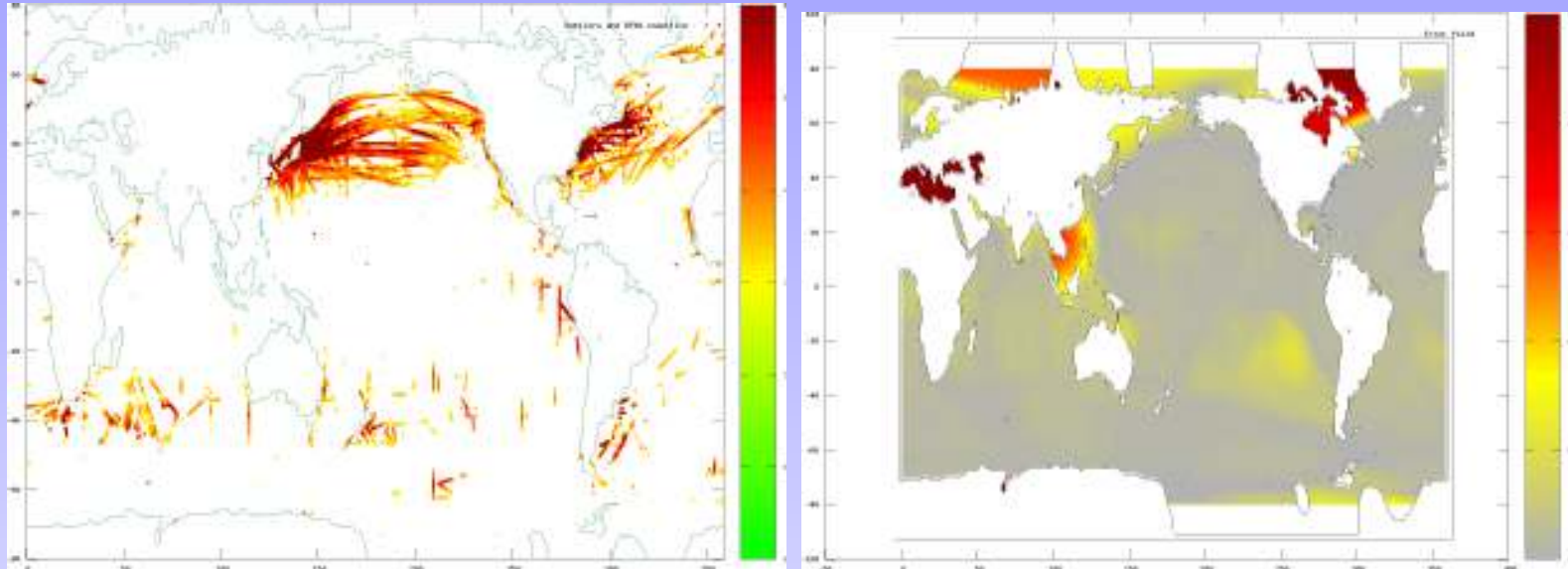


Huge problems

LDEO data base with $4.5 \cdot 10^6$ measurements (Takahashi *et al.*, 2009). Running on a laptop within a few minutes. Shown here, temperature fields.



Huge problems, outliers and relative error field

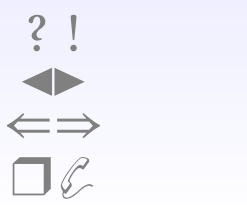
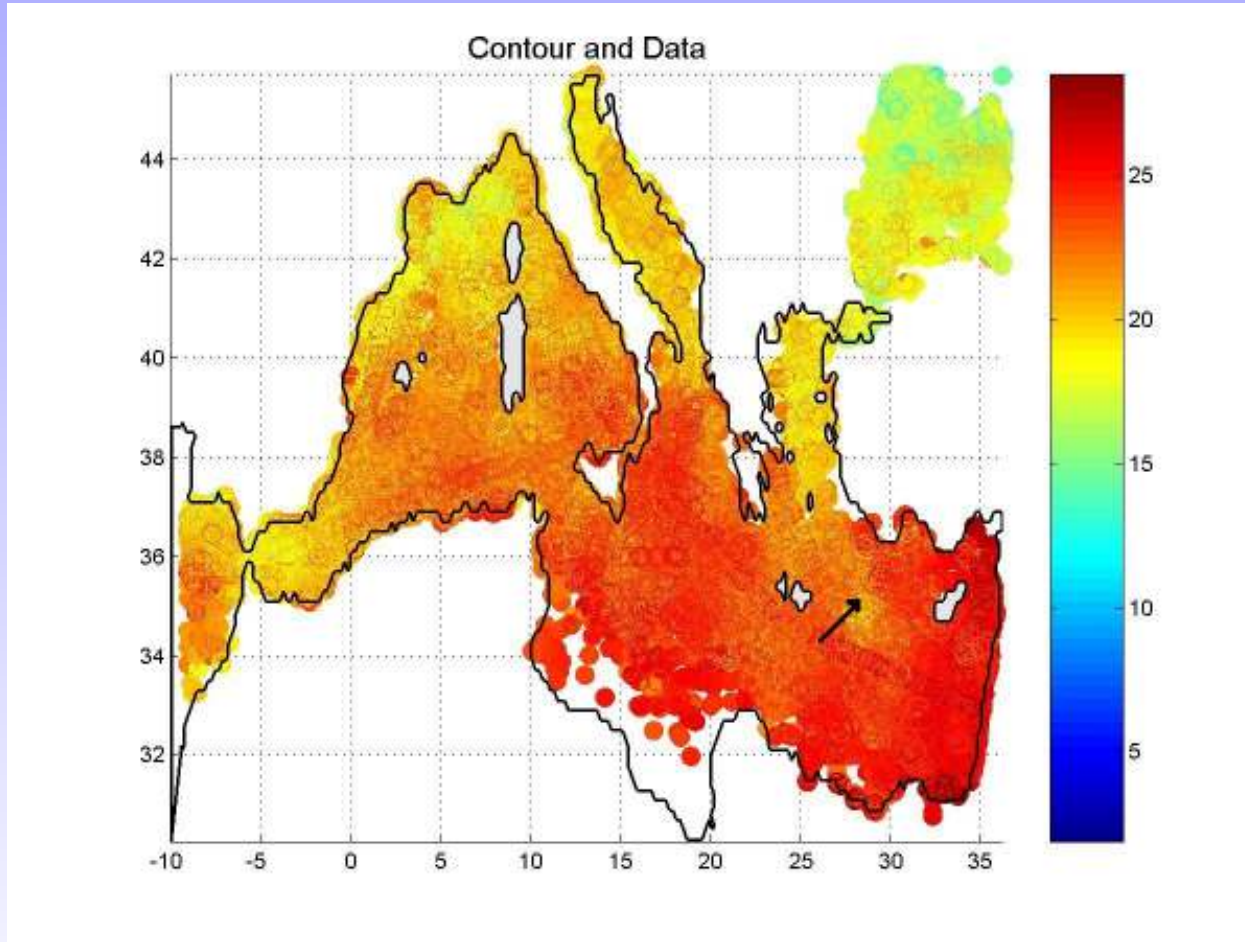


Outliers detected via comparison of statistically expected residuals (value provided by the DIVA analysis) and actual residuals (note that expected residuals decrease for large S/N).

Error field (on the right) can be used to mask regions with large uncertainties (low data coverage and/or large errors on data)

Outlier detection to detect encoding problems

Add value of 27 in 29°E , 35°N (21788th data point): corresponds to a displaced profile within a subregion

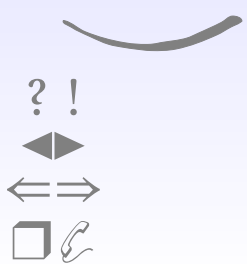


Outlier with *divaqc*

```

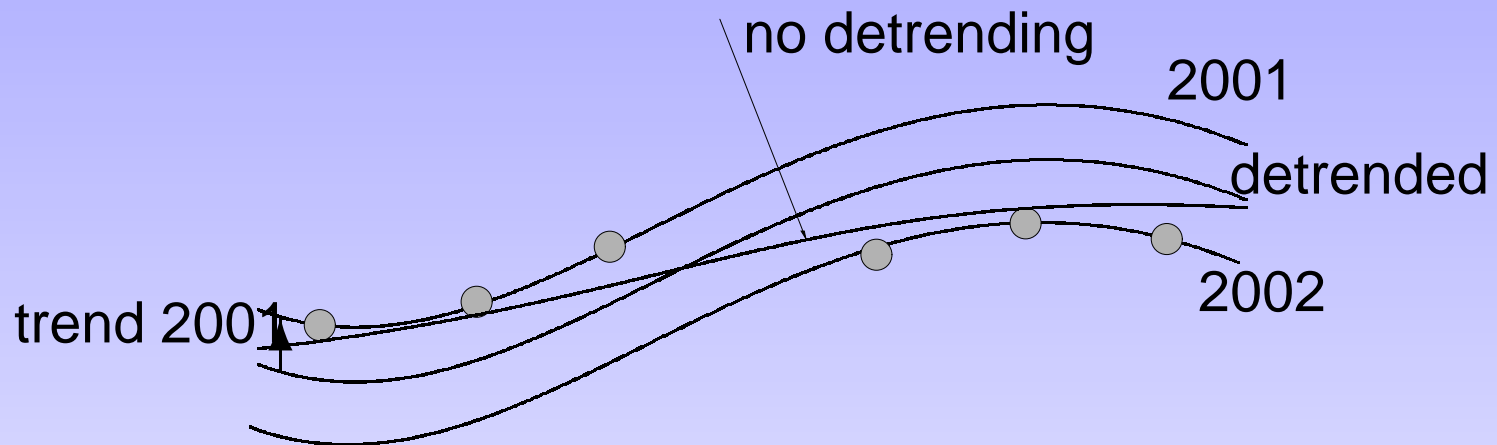
/cygdrive/c/jmb/cd-roms/modb/Utilities/Diva/Diva4.0/divastripped
Beckers@GHER22 /cygdrive/c/jmb/cd-roms/modb/Utilities/Diva/Diva4.0/divastripped
$ head -40 ./output/outliers.normalized.dat
7.83717633 6416 29. 33.6669998 13.7980003 23.3453999 0.696789324
7.75217195 2837 28.2999992 40.7750015 7.67000008 16.995903 0.688102722
7.42754382 6418 25.7666664 34.7669983 14.007 23.0623131 0.697402358
5.68016422 831 -0.773333311 37.7874985 27.6000004 20.6183472 0.699612796
4.35829445 20260 7.19999981 41.7999992 15.1000004 20.4000015 0.69670248
4.32356833 9578 7. 43.0666656 14. 19.3166256 0.704522073
4.26528099 822 -0.786666691 37.75 26. 20.7408123 0.701173782
4.25726546 460 -2.91333342 35.2050018 27.6000004 22.4128113 0.692871869
4.2435566 1379 6.0333333 42.8166656 13.8999996 19.1117496 0.703695774
4.23628475 21788 29. 35. 27. 21.8075123 0.697001696
4.23542502 18193 10.9666662 38. 17.7299995 22.9030018 0.699810088
4.15811381 18117 7. 43. 14.2299995 19.3404331 0.70424962
4.15148862 1524 7.3166666 43.6861649 14.7609997 19.8653717 0.704541206
4.13344054 8310 -0.781666696 36.4329987 15.1999998 20.2505627 0.700169802
4.06387505 828 -0.758333325 37.6833344 26. 20.9775677 0.702664018
4.05206397 825 -0.819999993 37.7050018 25.8999996 20.8979683 0.701841593
3.94206592 9927 4.2833333 42.8833351 15. 19.7462311 0.690053046
3.87482896 20258 7.43166685 40.0999985 16.6000004 21.26474 0.690022349
3.84992195 3213 6.5333333 41.3166656 15.5 20.1702461 0.695324957
3.80394796 1409 8.33333302 43.7999992 15.3800001 20.0317707 0.700980067
3.79860263 20263 7.19999981 42.9669991 14.8000002 19.4583645 0.702965677

```



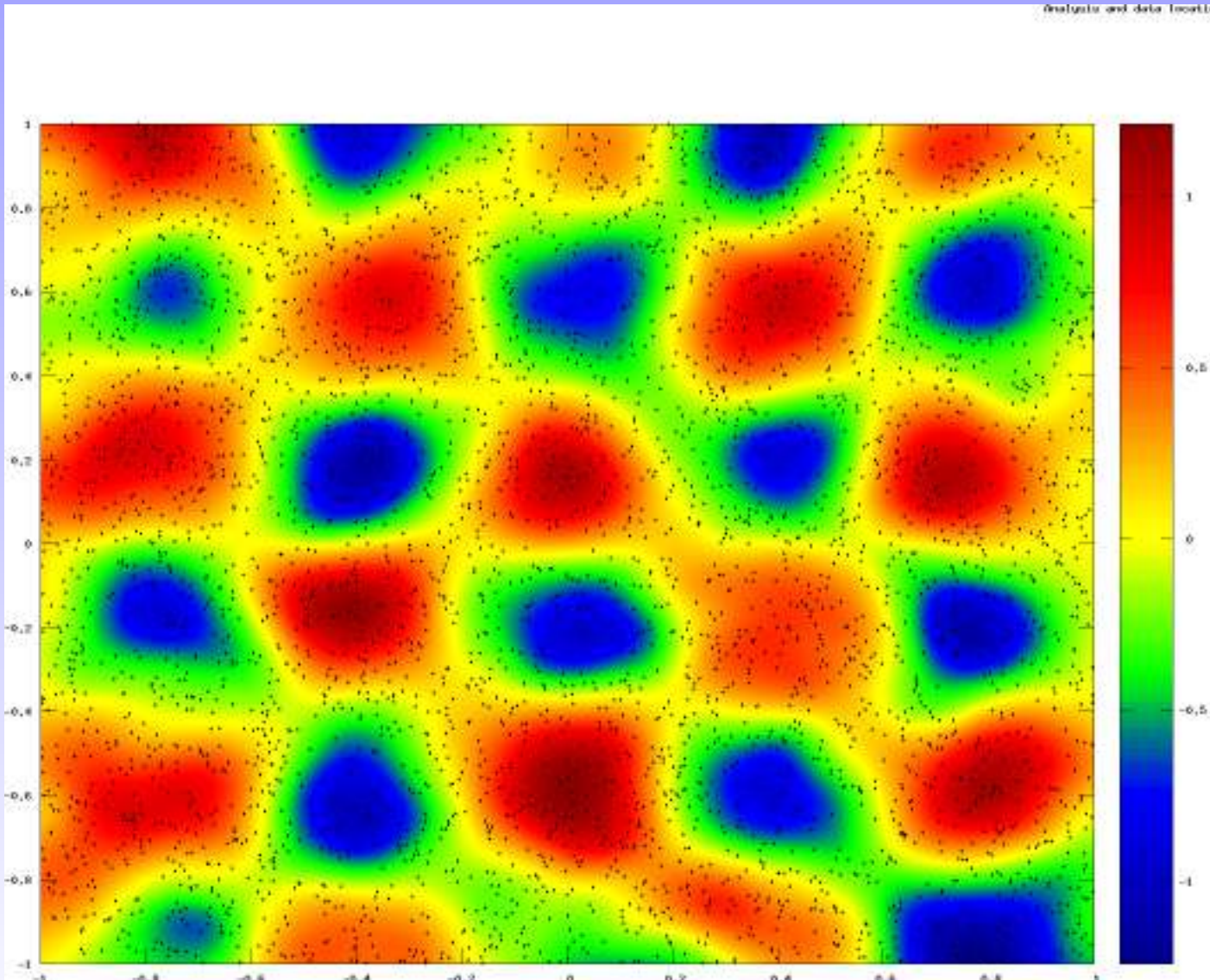
Detrending

Heterogeneous data distribution:



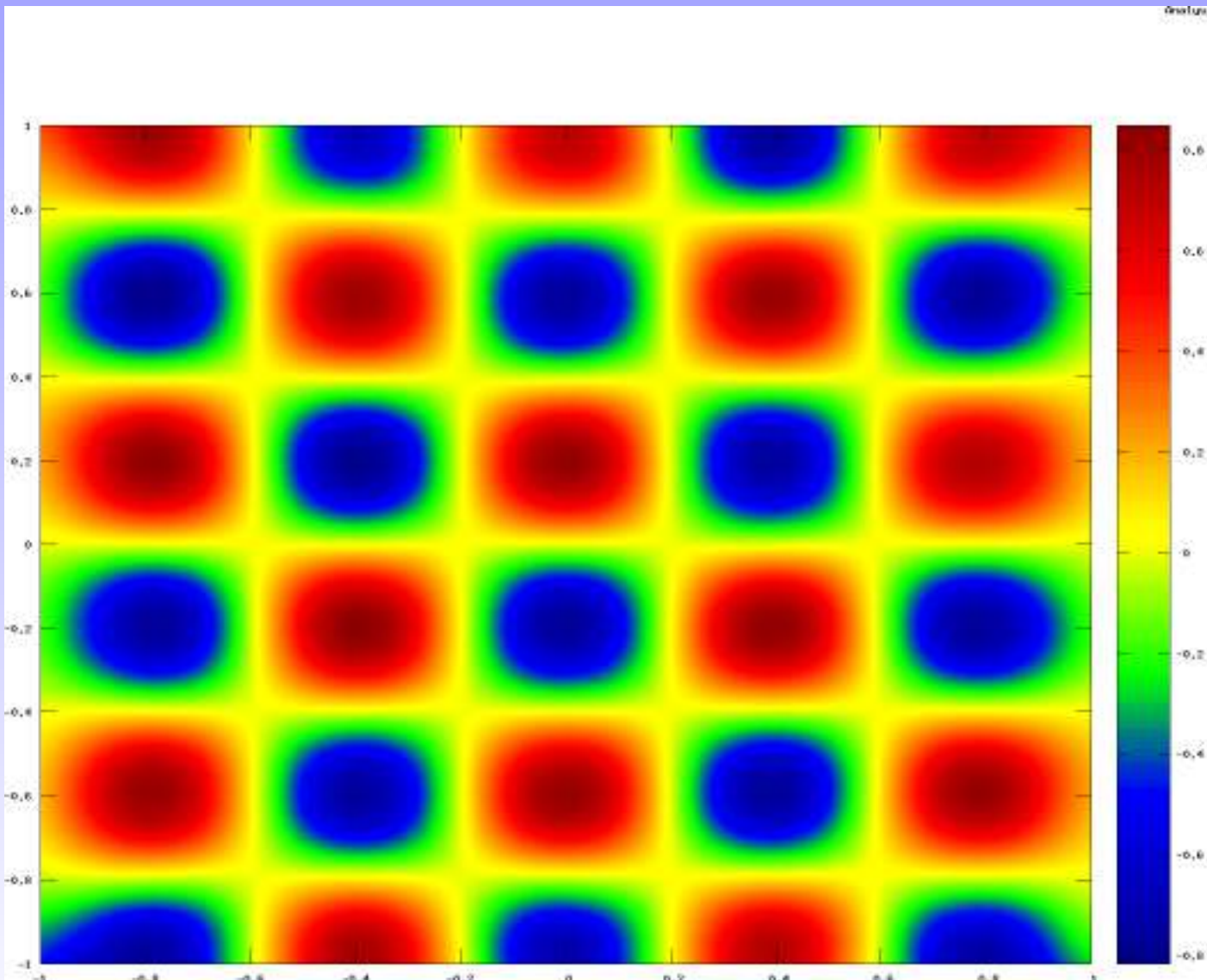
First analysis show a bias for each year's data with respect to first analysis. Subtract the bias estimate and redo the analysis, accumulating the bias. After convergence, detrended analysis+bias of the year.

Example without detrending



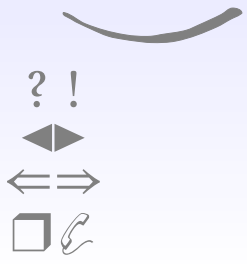
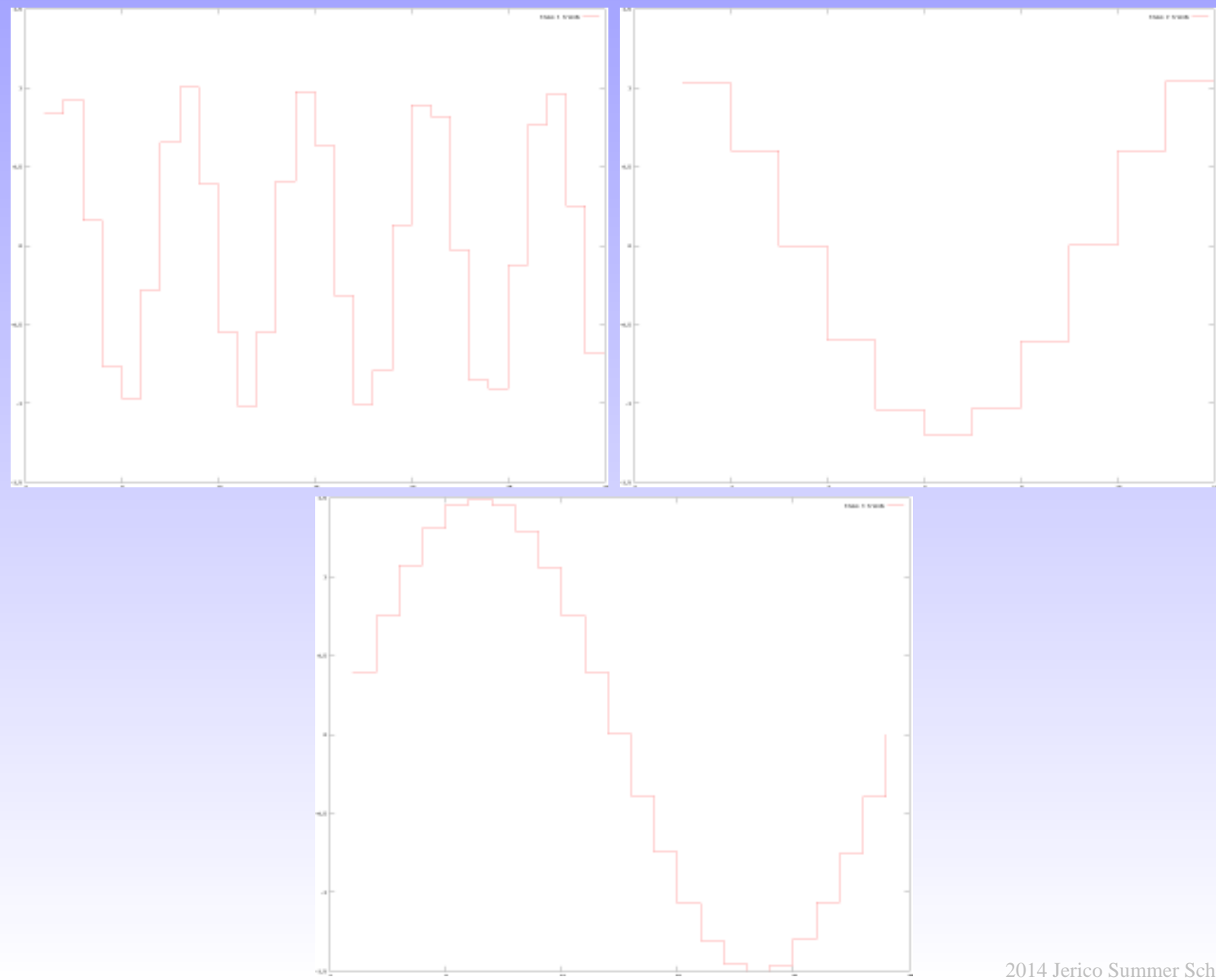
DIVA analysis of sin-cosine spatial structure with superimposed decadal, seasonal and daily cycles and noise.

Example with detrending

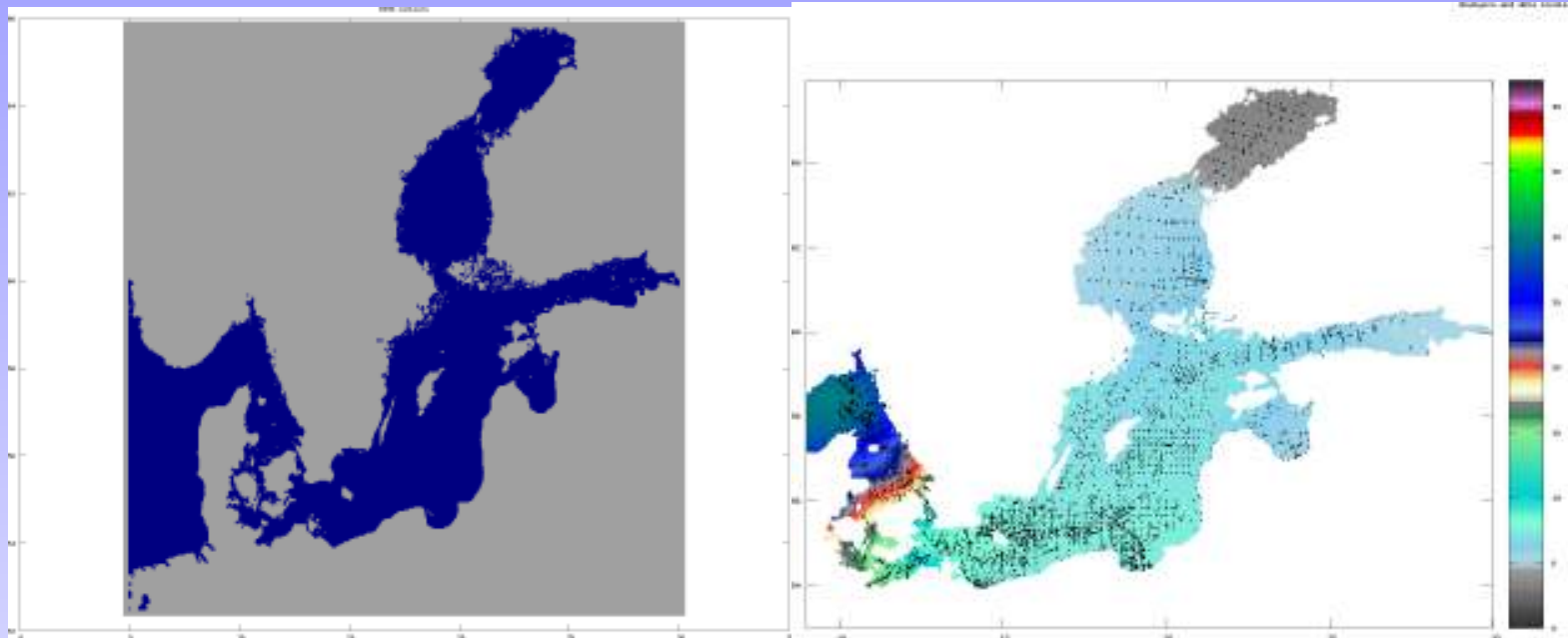


DIVA analysis of sin-cosine spatial structure with superimposed decadal, seasonal and daily cycles and noise.

Trends can also be retrieved

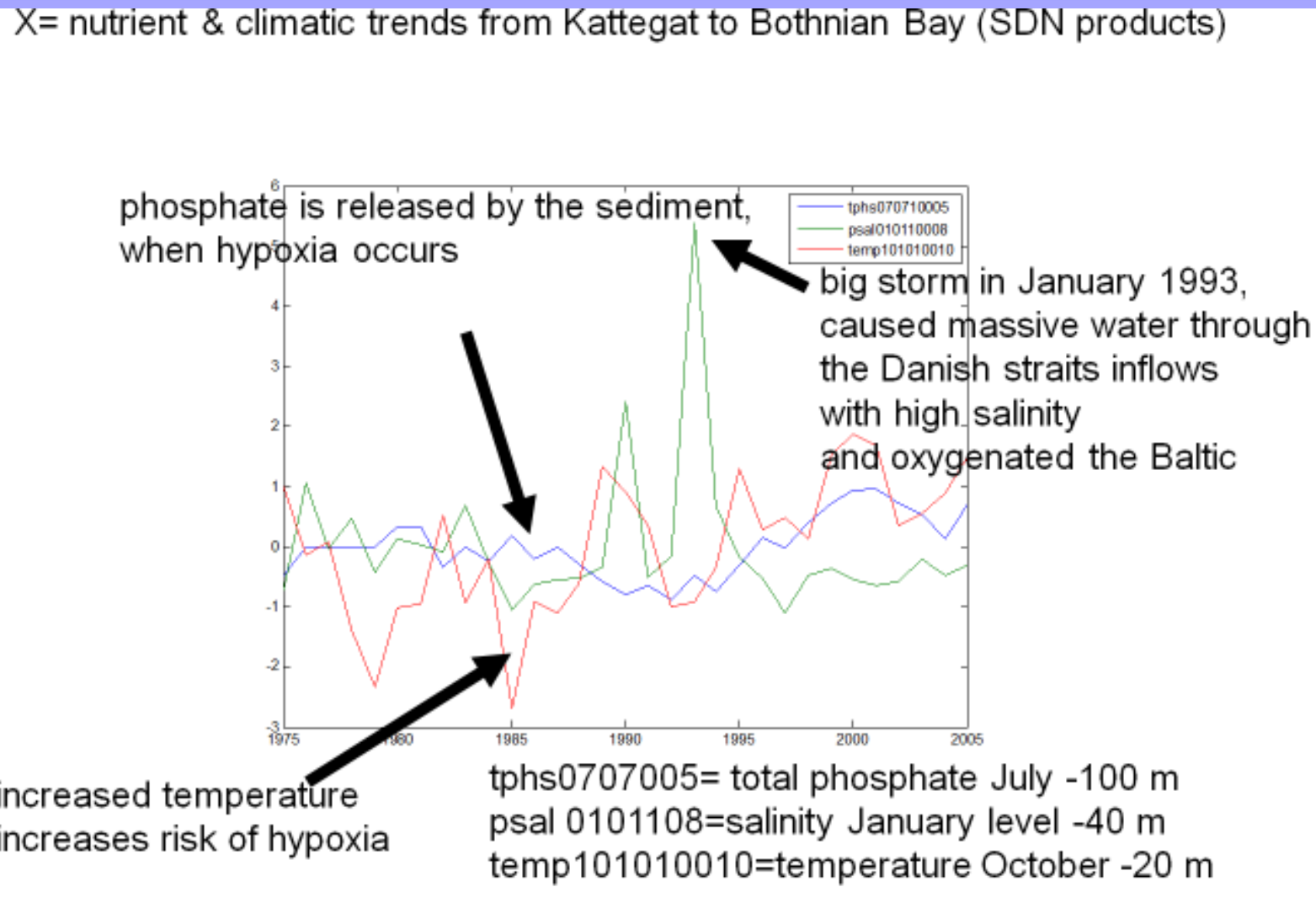


Heterogeneous case



Baltic Salinity Climatology (Bassompierre *et al.*, 2010)

Heterogeneous case, trends

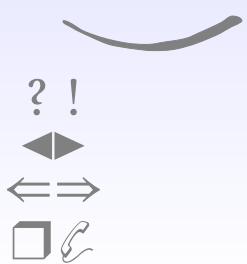


(Bassompierre *et al.*, 2010)

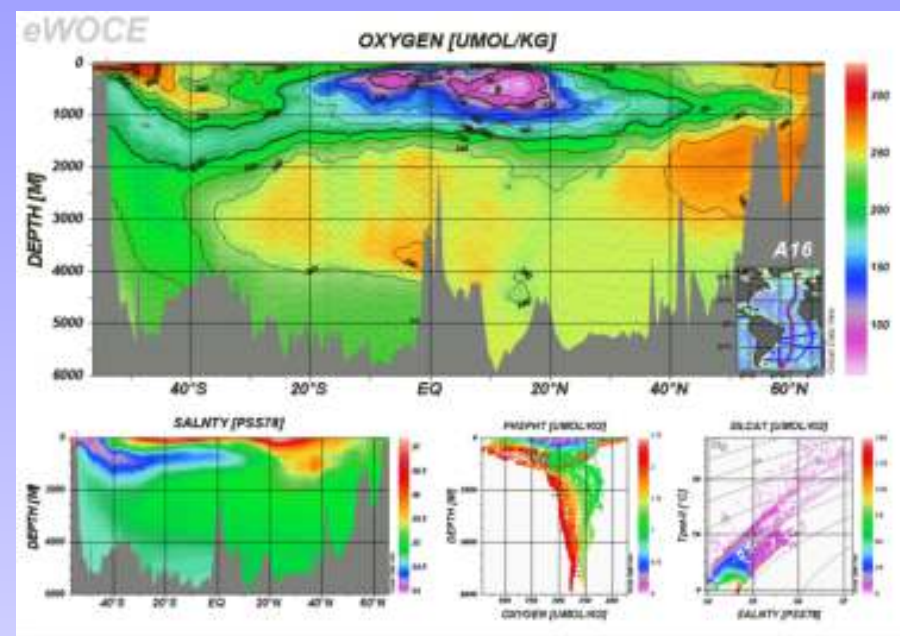


Université de Liège

- *Gridding*
- *DIVA theory*
- ***Implementations and exercises***
- *DINEOF theory*
- *Implementations and exercises*



How to use DIVA?



Analysis with Diva
 Correlation length [deg]:
 Signal to noise ratio:

Optional parameters
 Maximum rel. error (from 0 to 1):
 Range of color-bar (min,max):

Statistics Download analysis Link or embed Report a problem Help Properties
 13.67530, 34.66914

```

- (c:\pkr\c\job\new\diva-4.2.1\diva\diva)
CALL TO STORCS MODULE: IPR = 1
#####
Total no. of pts where gridded solution is asked = 19201
Finished storing
#####
CALL TO SCIFAC MODULE: IPR = 1
#####
Trace average estimate = 0.0139772668
max of points = 1.3259107
MAXIMUM NUMBER OF SINTERES USED = 152895
MAXIMUM NUMBER OF REAL USED = 6776828
PRIOR ESTIMATE OF SINTERES USED = 480230
PRIOR ESTIMATE OF REAL USED = 9522239
#####
2.1.0.0 -> 4.2.1 - Execution Completed +
#####
Output of results for user
Fort 04 -> ./output/fieldgher.nc
Fort 02 -> ./output/walstisqacis.nc
Fort 03 -> ./output/fieldascii.nc
Fort 07 -> ./output/errorfieldgher.nc
Fort 06 -> ./output/errorfieldascii.nc
Fort 11 -> ./output/fieldststapoint.nc
Fort 77 -> ./output/gouval.dat

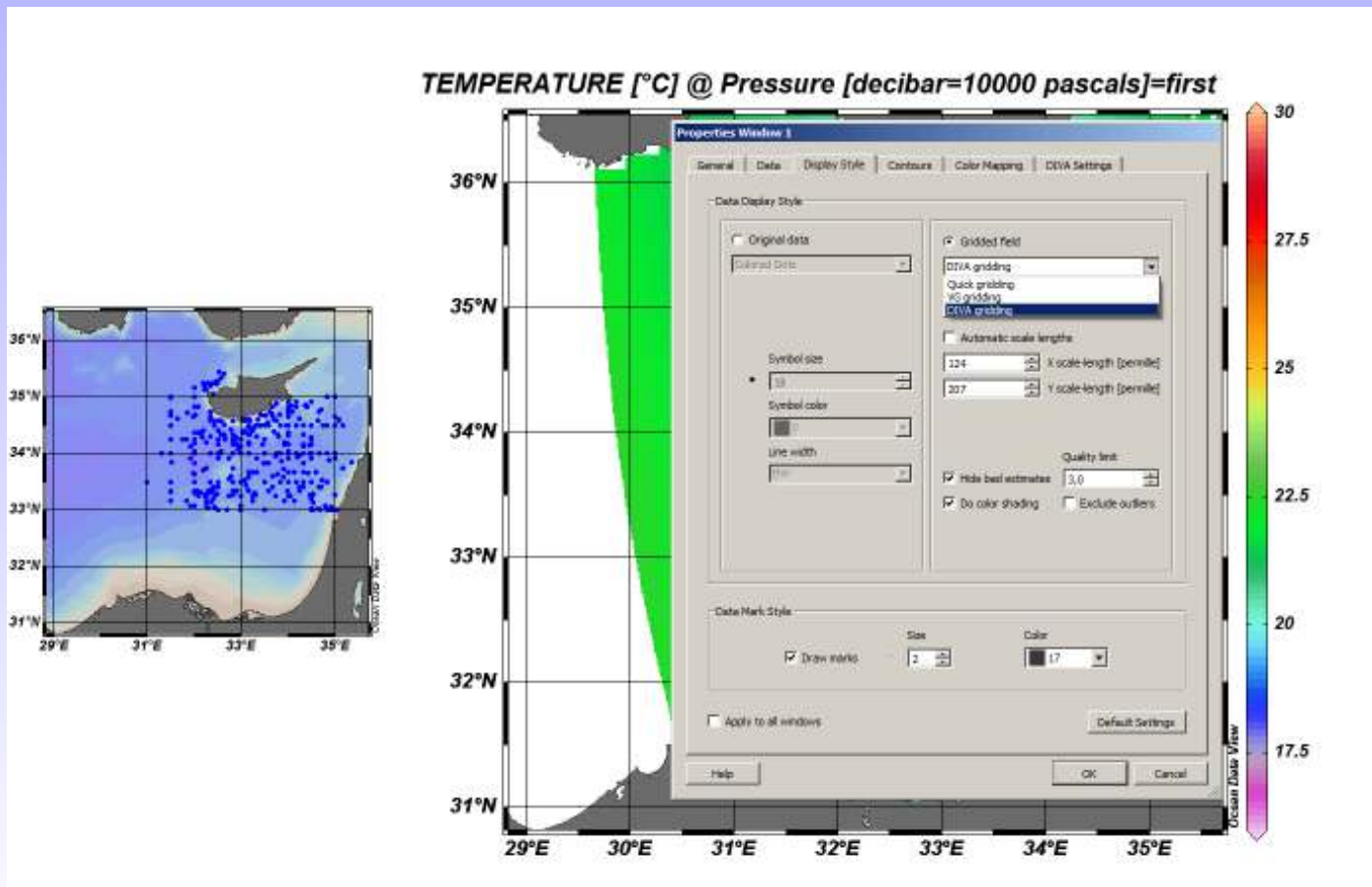
Creation of file GridInfo.dat
Fort 07 -> ./output/ghertonatcdf/fort.07
(creating netcdf file only for field
since Warbac and lopec are 1 0
*** SUCCESS writing NetCDF file results.nc
#####
Analysis is finished
#####
Dec 09 09:03:23 /c:/pkr/c/job/cr/ross/diva4.2.1/diva\diva
  
```



Try parameters of gridding in ODV

On Display Style

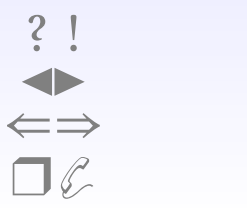
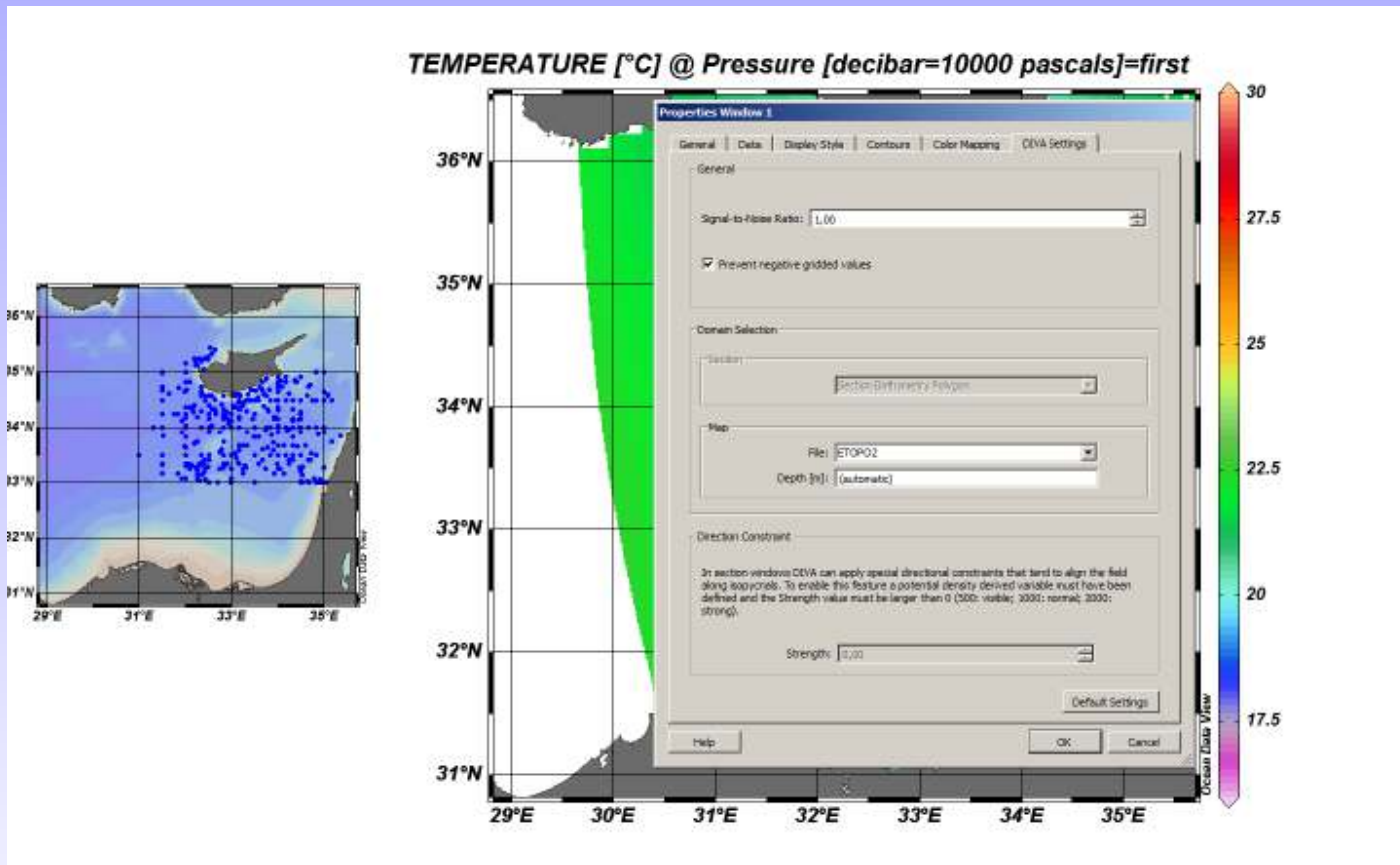
- change analysis method (quick, VG, DIVA)
- change X scale-length and Y scale-length



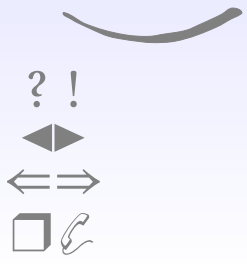
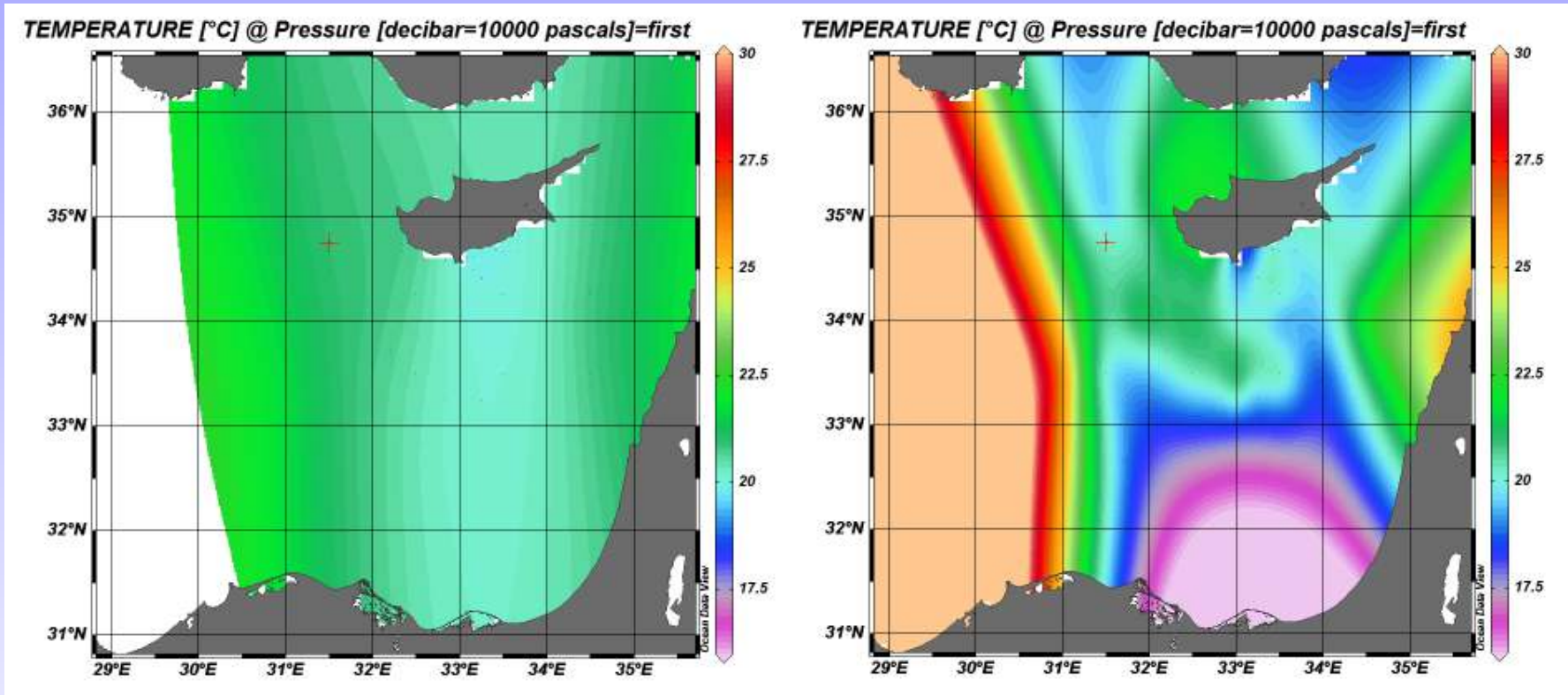
Try parameters of gridding in ODV

On DIVA Settings

- Change Signal-to-Noise Ratio



Observed changes in analyses due to changes in parameters (here signal-to-noise ratio from 1 to 100)



Diva-on-web

<http://gher-diva.phys.ulg.ac.be/web-vis/diva.html>

Upload Grid Analysis Statistics Download analysis Link or embed Report a problem Help

Upload observation

Text file ODV4

File:

Column separator:

Decimal separator:

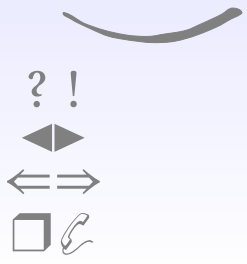
Format

The file must be an ASCII text file with three columns. The columns represent longitude, latitude and value of the observation respectively. For example:

```
29.7667 45.15 16.146
29.7667 45.15 16.346
...
```

[Sample global temperature data from ARGO](#)

180.70313, -123.04688



Diva-on-web

Data upload (3 column ascii file or ODV4) and output grid definition

The screenshot shows the 'Grid' configuration panel on the left and a map view on the right. The 'Grid' panel includes the following fields:

- Longitude resolution:
- Latitude resolution:
- Longitude range:
- Latitude range:
- Depth level (m):
- Bathymetric data base:

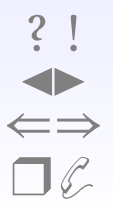
Buttons: 'Previous' and 'Next' are located at the bottom of the grid panel. The map view on the right shows a satellite-style map of the North Atlantic region with a grid overlay. A legend on the right side of the map includes:

- Base Layer
 - GEBCO
 - NASA Blue marble
 - Metacarta
 - Land-sea mask
 - 0 m isobath
- Overlays
 - Location of observations

Map navigation controls (pan, zoom) are visible on the left side of the map. A coordinate box in the bottom right corner of the map displays: -1.40275, 61.99181.



Université de Liège



Diva-on-web

Analysis parameter definition (or fit)

Université de Liège

Upload | Grid | **Analysis** | Statistics | Download analysis | Link or embed | Report a problem | Help


Analysis with Diva

Correlation length [deg]:
Signal to noise ratio:

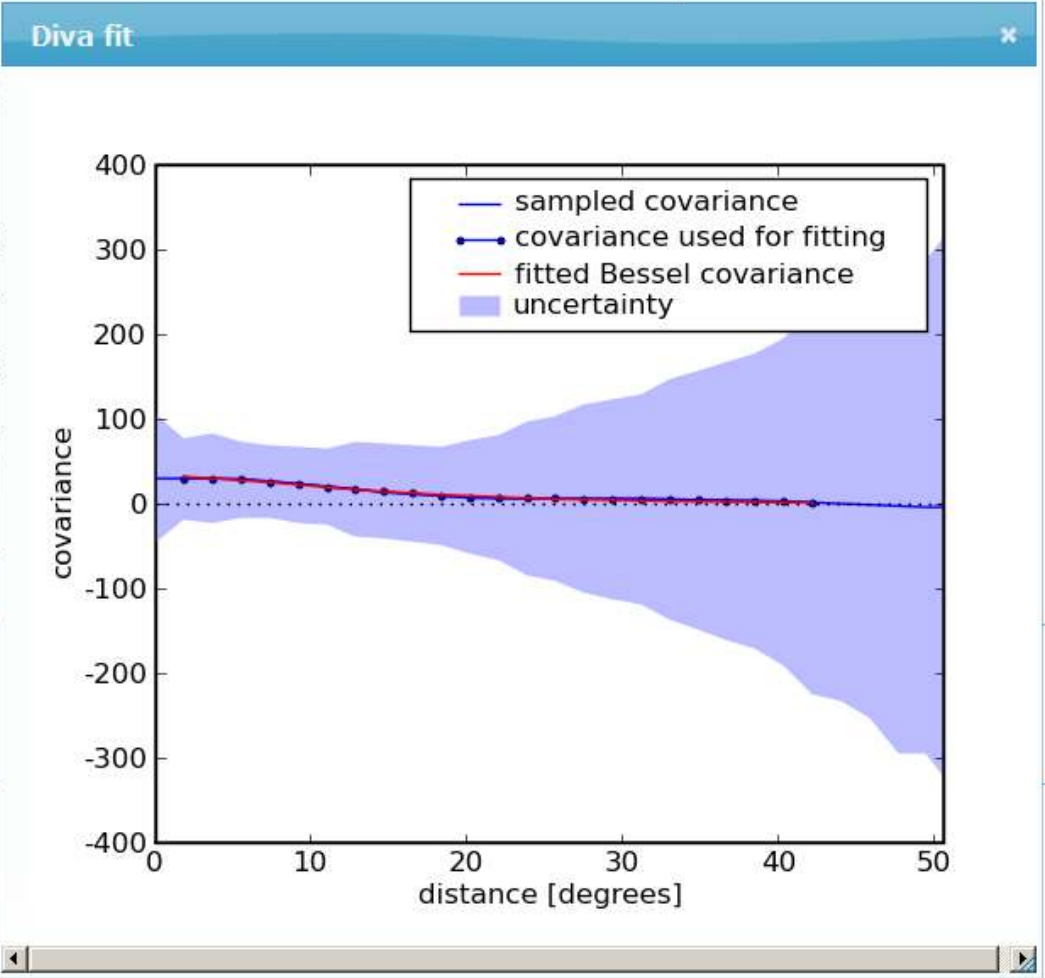
Quality of the fit (0: bad 1: good): 0.963967


Optional parameters

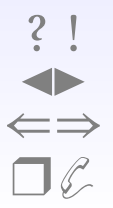
Maximum rel. error (from 0 to 1):



Diva fit







Diva-on-web

Analysis (and numerical grid)

Upload | Grid | **Analysis**

Statistics | Download analysis | Link or embed | Report a problem | Help

Analysis with Diva

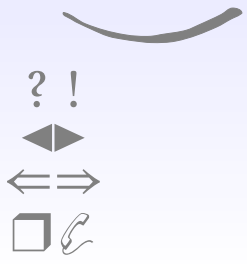
Correlation length [deg]:
Signal to noise ratio:

Quality of the fit (0: bad 1: good):
0.963967

Optional parameters

Maximum rel. error (from 0 to 1):

44.64844, 30.17578



Diva-on-web

Plotting options

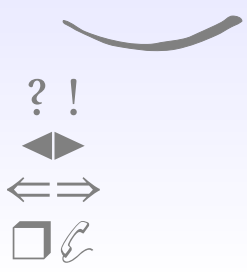
The screenshot displays the 'Analysis with Diva' interface. On the left, the 'Analysis' tab is active, showing the following data:

- Correlation length [deg]: 10.3516
- Signal to noise ratio: 1.08679
- Quality of the fit (0: bad 1: good): 0.963967
- Optional parameters: Maximum rel. error (from 0 to 1): 0.3

The central panel shows a global map with a color-coded data distribution. A vertical color bar on the right indicates values from 15 to 30. A 'Configuration' dialog box is open on the right side, with the following settings:

- Colormap: (rainbow color bar)
- Invert colormap:
- Plotting style: Flat shading
- Minimum color-bar range: 0
- Maximum color-bar range: 30
- Number of contour-lines: 40

Buttons for 'Reset to default' and 'Close' are visible at the bottom of the configuration dialog. The bottom of the interface features logos for GHER, SeaDataNet, and Diva.



Diva-on-web

Download options

The screenshot shows the 'Analysis with Diva' interface. At the top, there are tabs for 'Upload', 'Grid', and 'Analysis'. A secondary row of buttons includes 'Statistics', 'Download analysis', 'Link or embed', 'Report a problem', and 'Help'. The main panel displays analysis results: 'Correlation length [deg]: 10.3516', 'Signal to noise ratio: 1.08679', and 'Quality of the fit (0: bad 1: good): 0.963967'. Below this, 'Optional parameters' shows 'Maximum rel. error (from 0 to 1): 0.3'. A 'Download' dialog box is open, listing available formats: NetCDF file (.nc), Octave or Matlab (.mat), Google Earth (.kml), and Image Format. The 'Image Format' dropdown menu is expanded, showing options for PNG, PDF, EPS, and SVG. A map in the background shows a coastal area with a color scale from 24 to 30. The bottom of the interface features logos for GHER, SeaDataNet, and DIVA.



Diva-on-web

Exploitation of WMS-OGC layering techniques

Université de Liège



Upload Grid Analysis Statistics Download analysis Link or embed Report a problem Help

Analysis with Diva

Correlation length [deg]:
Signal to noise ratio:

Quality of the fit (0: bad 1: good):

Optional parameters

Maximum rel. error (from 0 to 1):

Link or embed in your web site

Link:

Embed:

Copy and paste this line of code in your web page. To keep your results on our web-server, you must click on save below. We would appreciate if you leave your name and email address [\[more\]](#).

Name:

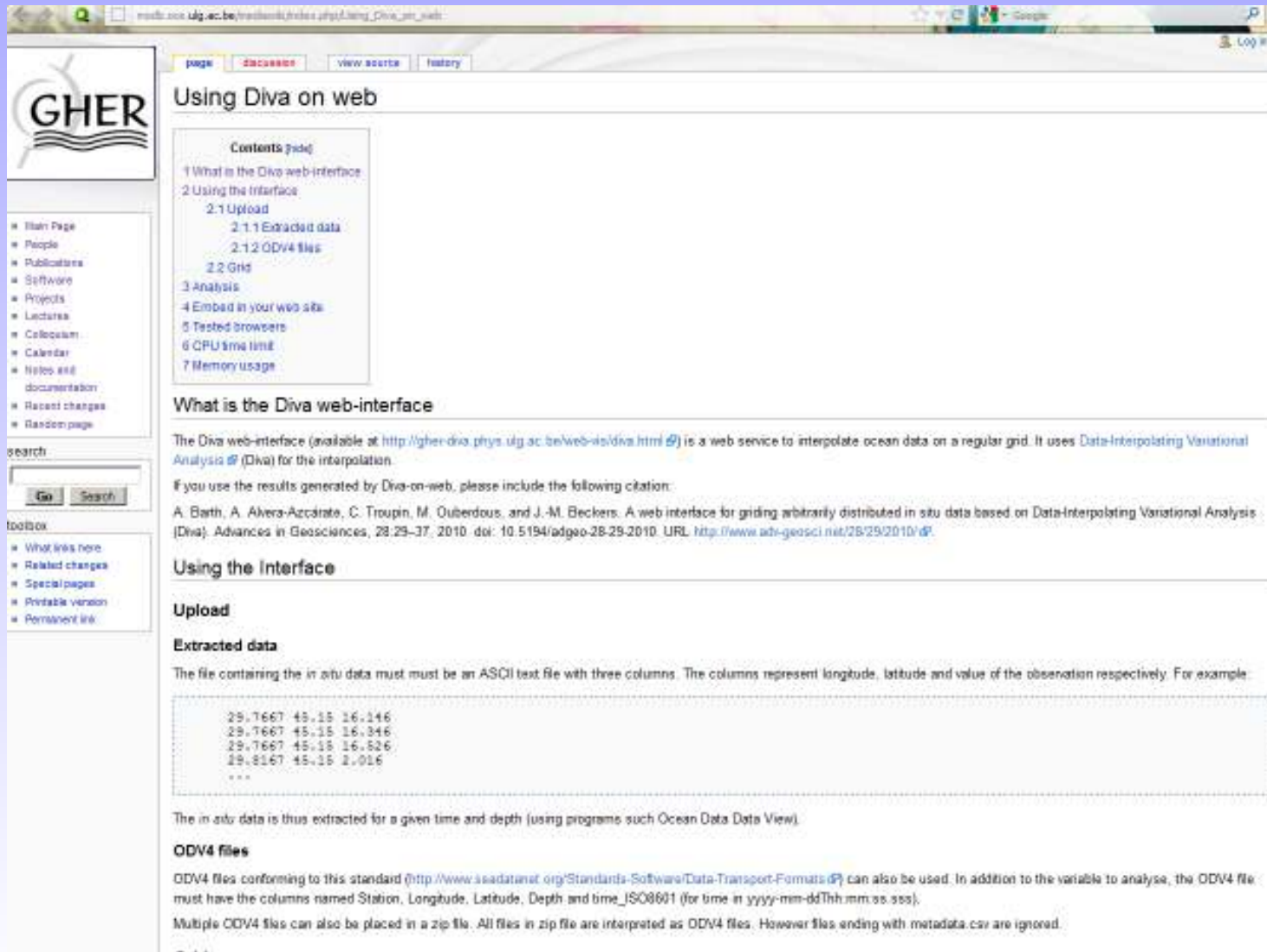
Email:



Help

More information

http://modb.oce.ulg.ac.be/mediawiki/index.php/Using_Diva_on_web



The screenshot shows a web browser window displaying the GHER Diva web interface help page. The page title is "Using Diva on web". It features a navigation menu on the left with links like "Main Page", "People", "Publications", "Software", "Projects", "Lectures", "Colloquium", "Calendar", "Help and documentation", "Recent changes", and "Random page". Below the menu is a search box and a toolbox with links for "What links here", "Related changes", "Special pages", "Printable version", and "Permanent link". The main content area includes a "Contents" table of contents, a section titled "What is the Diva web-interface" with a description and citation, a section titled "Using the interface", and a section titled "Upload" with a sub-section "Extracted data" showing an example of ASCII text data for in-situ observations.

Contents (hide)

- 1 What is the Diva web-interface
- 2 Using the interface
 - 2.1 Upload
 - 2.1.1 Extracted data
 - 2.1.2 ODV4 files
 - 2.2 Grids
- 3 Analysis
- 4 Embed in your web site
- 5 Tested browsers
- 6 CPU time limit
- 7 Memory usage

What is the Diva web-interface

The Diva web-interface (available at <http://gher-diva.phys.ulg.ac.be/web-visit/diva.html>) is a web service to interpolate ocean data on a regular grid. It uses Data-Interpolating Variational Analysis (DIVA) for the interpolation.

If you use the results generated by Diva-on-web, please include the following citation:

A. Barth, A. Akera-Azzdrate, C. Troupin, M. Ouberdous, and J.-M. Beckers. A web interface for gridding arbitrarily distributed in situ data based on Data-Interpolating Variational Analysis (DIVA). *Advances in Geosciences*, 28:29–37, 2010. doi: 10.5194/adgeo-28-29-2010. URL <http://www.adv-geosci.net/28/29/2010/>.

Using the interface

Upload

Extracted data

The file containing the in situ data must be an ASCII text file with three columns. The columns represent longitude, latitude and value of the observation respectively. For example:

```

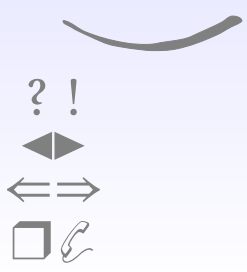
29.7667 45.15 16.146
29.7667 45.15 16.346
29.7667 45.15 16.526
29.8167 45.15 2.016
...

```

The in situ data is thus extracted for a given time and depth (using programs such as Ocean Data Data View).

ODV4 files

ODV4 files conforming to this standard (<http://www.seadatanet.org/Standards-Software/Data-Transport-Formats>) can also be used. In addition to the variable to analyse, the ODV4 file must have the columns named Station, Longitude, Latitude, Depth and time_ISO8601 (for time in yyyy-mm-ddThh:mm:ss.sss). Multiple ODV4 files can also be placed in a zip file. All files in zip file are interpreted as ODV4 files. However files ending with metadata.csv are ignored.



Software download for advanced users: **GODIVA 4D**

<http://modb.oce.ulg.ac.be/mediawiki/index.php/DIVA>

GHER

DIVA

DIVA allows the spatial interpolation of data (analysis) in an optimal way, comparable to optimal interpolation (OI). In comparison to OI it takes into account coastlines, sub-basins and advection. Calculations are highly optimized and rely on a finite element resolution. Tools to generate the finite element mesh are provided as well as tools to optimize the parameters of the analysis. Quality control of data can be performed and error fields can be calculated. Also detrending of data is possible. Finally 3D and 4D extensions are included with emphasis on direct computations of climatologies from COV2 spreadsheet files.

The research leading to the development of DIVA has received funding from the European Union Seventh Framework Programme (FP7/2007-2013) under grant agreement n°283607, [SeaDataNet 2d](#).

Contents (hide)

- 1 In a few words
- 2 How to get the code?
- 3 User workshops
- 4 The method
- 5 Publications & documents
- 6 Matlab/Octave tools
- 7 Quality control of products
- 8 Testing new versions
- 9 SVN commands for Diva

In a few words

Diva is a software developed for gridding in situ data.

It uses a finite-element method¹ to solve a variational principle which takes into account:

1. the distance between analysis and data (observation constraint),
2. the regularity of the analysis (smoothness constraint).

GODIVA

Command line version:

<http://modb.oce.ulg.ac.be/mediawiki/index.php/DIVA>
currently version 4.6.5

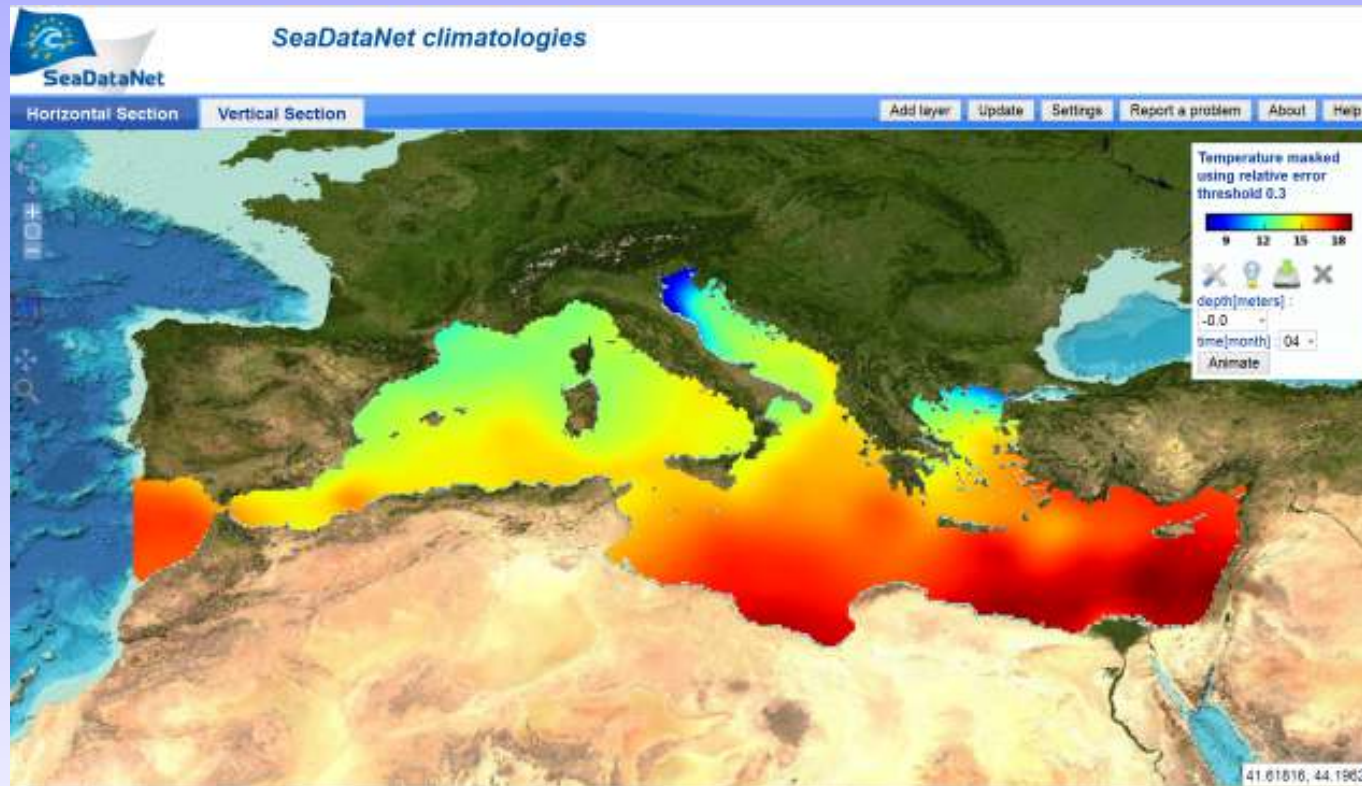
- All features
- Customizable
- Automatized
- Linux or Cygwin needed
- A few driver files allow automatic creation of climatologies using ODV files.
- Recent developments: parallel solver, more efficient grid generator, approximate and quick error calculations...

Google user group


http://groups.google.com/group/diva_users for
feedback, questions, suggestions etc; developer's contribution via
SVN

OceanBrowser


Results of GODIVA (4D netCDF files with CF conventions), ready for upload on server with OceanBrowser visualization (including vertical sections). OGC-WMS approach.




<http://gher-diva.phys.ulg.ac.be/web-vis/>


 P. Brasseur, J.-M. Beckers, J.-M. Brankart, and R. Schoenauen. Seasonal temperature and salinity fields in the Mediterranean Sea: Climatological analyses of a historical data set. *Deep Sea Research*, 43:159–192, 1996.


<http://orbi.ulg.ac.be/handle/2268/4788>

 Ch. Troupin, F. Machin, M. Ouberdous, D. Sirjacobs, A. Barth, J.-M. Beckers. High-resolution Climatology of the North-East Atlantic using Data-Interpolating Variational Analysis (Diva). *Journal of Geophysical Research*, 114, 2010.


<http://orbi.ulg.ac.be/handle/2268/68400>

 M. Rixen, J.-M. Beckers, J.-M. Brankart, and P. Brasseur. A numerically efficient data analysis method with error map generation. *Ocean Modelling*, 2:45–60, 2000. <http://orbi.ulg.ac.be/handle/2268/40371>

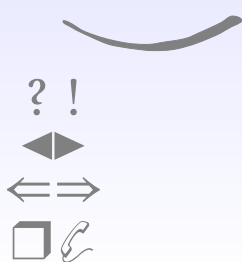
 A. Karafistan, J.-M. Martin, M. Rixen, and J.-M. Beckers. Space and time distributions of phosphates in the Mediterranean Sea. *Deep Sea Research*, 49:67–82, 2002. <http://orbi.ulg.ac.be/handle/2268/4289>


 Tyberghein, L., Verbruggen, H., Klaas, P., Troupin, C., Mineur, F., De Clerck, O., 2011. ORACLE: a global environmental dataset for marine species distribution modeling. *Global Ecology and Biogeography*.

<http://orbi.ulg.ac.be/handle/2268/112937>


 Barth, A., Alvera-Azcárate, A., Troupin, C., Ouberdous, M., Beckers, J.M., 2010. A web interface for gridding arbitrarily distributed in situ data based on Data-Interpolating Variational Analysis (DIVA). *Adv. Geosci.* 28, 29-37.

<http://orbi.ulg.ac.be/handle/2268/81401>



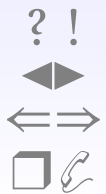
 M. Rixen, J.-M. Beckers, S. Levitus, J. Antonov, T. Boyer, C. Maillard, M. Fichaut, E. Balopoulos, S. Iona, H. Dooley, M.-J. Garcia, B. Manca, A. Giorgetti, G. Manzella, N. Mikhailov, N. Pinardi, M. Zavatarelli, and the Medar Consortium. The Western Mediterranean Deep Water: a proxy for global climate change. *Geophysical Research Letters*, 32, 2005.

<http://orbi.ulg.ac.be/handle/2268/4299>

 C. Troupin, A. Barth, D. Sirjacobs, M. Ouberdous, J.-M. Brankart, P. Brasseur, M. Rixen, A. Alvera-Azcárate, M. Belounis, A. Capet, F. Lenartz, M.-E. Toussaint, J.-M. Beckers. Generation of analysis and consistent error fields using the Data Interpolating Variational Analysis (DIVA). *Ocean Modelling*, 52, 90-101, 2012.

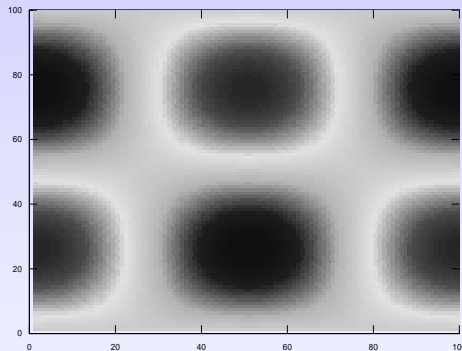
<http://orbi.ulg.ac.be/handle/2268/125731>

- *Gridding*
- *DIVA theory*
- *Implementations and exercises*
- ***DINEOF theory***
- *Implementations and exercises*

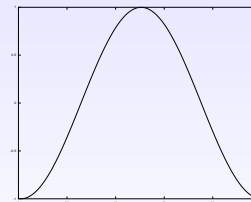


EOFs: Generalisations and other names

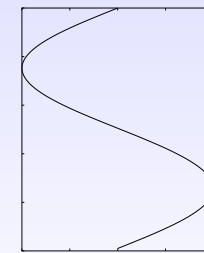
- Empirical orthogonal functions (EOFs)
- Proper orthogonal decomposition (POD)
- Karhunen-Loève decompositions (best to start from for non-uniform data distribution)
- Proper orthogonal modes (POM)
- Principal component analysis (PCA)



=



x



Classical approach for EOFs

- We assume that we have a matrix \mathbf{X} containing the observations, which is arranged such that the element i, j of the matrix is called $(\mathbf{X})_{ij}$ and is given by the value of the field $f(\mathbf{r}, t)$ at location \mathbf{r}_i and moment t_j :

$$(\mathbf{X})_{ij} = f(\mathbf{r}_i, t_j). \quad (45)$$

- The field f is an observational field and contains thus all errors (instrumental, unresolved structures, etc).
- We can then write the matrix as a succession of n column vectors

$$\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n), \quad (46)$$

each of the column vectors \mathbf{x}_j being the discrete state vector of size m at moment t_j .

Defining a mode

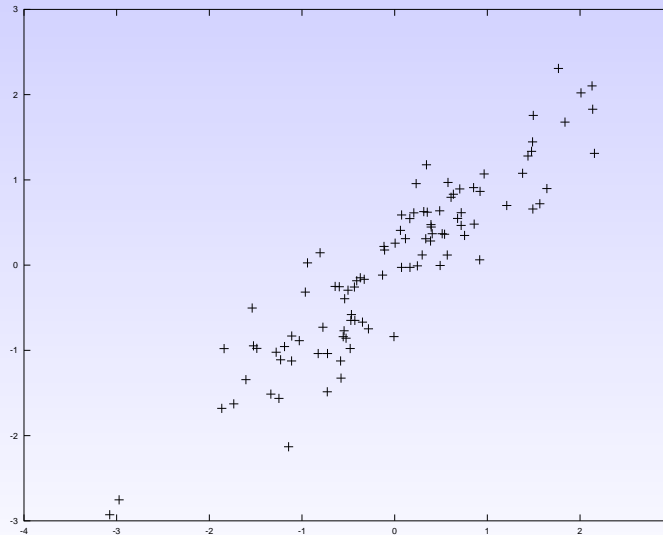
Try to find a spatial structure \mathbf{u} which represents at best the data:

Maximize norm of $\mathbf{X}^* \mathbf{u}$ with normalization constraint on \mathbf{u} .

Try to find the direction in which the data have their largest component.

Find extrema of functional J with Lagrange multiplier

$$J = \mathbf{u}^* \mathbf{X} \mathbf{X}^* \mathbf{u} - \lambda (\mathbf{u}^* \mathbf{u} - 1) \quad (47)$$



Euler-Lagrange equation

- Variations in (47) on \mathbf{u} :

$$\mathbf{X}\mathbf{X}^* \mathbf{u} = \lambda \mathbf{u} \quad (48)$$

- Variations on λ

$$\mathbf{u}^* \mathbf{u} = 1 \quad (49)$$

EOFs are normalized eigenvectors of "covariance"^a matrix $\mathbf{X}\mathbf{X}^*$ which is a symmetric positive defined matrix: real positive eigenvalues and orthogonal eigenvectors:

$$\lambda_i = \rho_i^2 \quad \text{conventionally } \rho_i > 0 \text{ and } \rho_{i+1} \leq \rho_i \quad (50)$$

$$\mathbf{u}_i^* \mathbf{u}_j = \delta_{ij} \quad (51)$$

Storing \mathbf{u}_i as columns in \mathbf{U} yields $\mathbf{U}^* \mathbf{U} = \mathbf{I}$

^a " " because missing 1/n. Observe time summation to get spatial covariances

Temporal amplitudes

What is the temporal evolution g_j of the amplitudes of a mode u_j ?

Temporal amplitudes

What is the temporal evolution g_j of the amplitudes of a mode u_j ?
See it as minimizing the norm of $\mathbf{X} - u_j g_j^*$

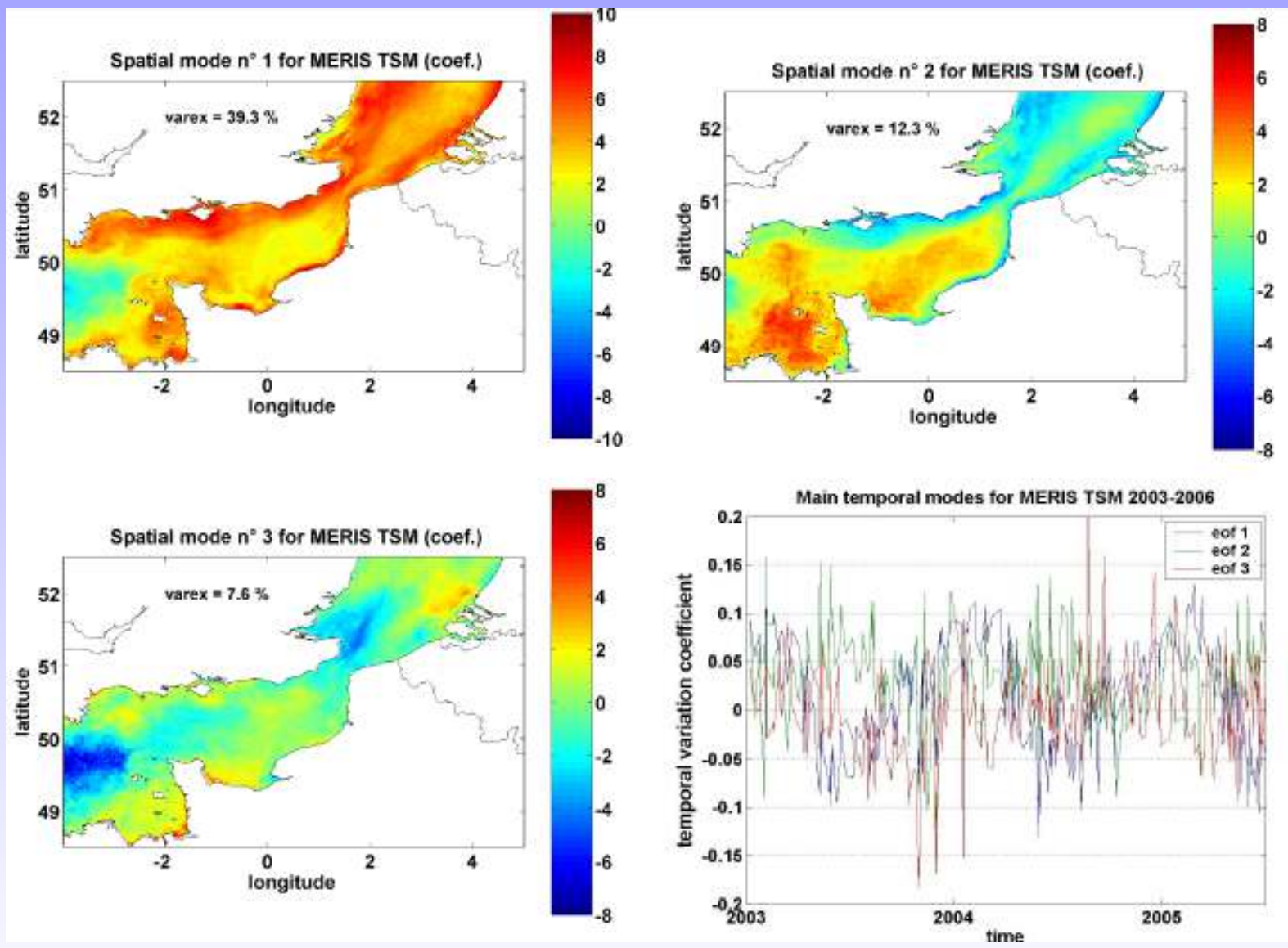
Temporal amplitudes

What is the temporal evolution g_j of the amplitudes of a mode u_j ?
 See it as minimizing the norm of $\mathbf{X} - u_j g_j^*$

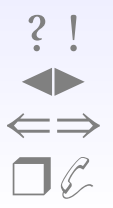
$$g_j = \mathbf{X}^* u_j \quad (52)$$

Projection of data of a given moment onto the spatial mode u_j

Example of EOF



Université de Liège



Temporal modes

Using temporal covariances $\mathbf{X}^* \mathbf{X}$ instead of spatial covariances $\mathbf{X} \mathbf{X}^*$ yields temporal EOFs :

$$\mathbf{X}^* \mathbf{X} \mathbf{v} = \mu \mathbf{v} \quad (53)$$

$$\mathbf{v}^* \mathbf{v} = 1 \quad (54)$$

$$\mathbf{V}^* \mathbf{V} = \mathbf{I} \quad (55)$$

Link between projection of data and temporal modes? Yes,

$$\mathbf{g}_j = \mathbf{X}^* \mathbf{u}_j = \rho_j \mathbf{v}_j \quad (56)$$

easily proven via SVD decomposition of a matrix

SVD

Singular value decomposition of a data matrix \mathbf{X} :

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^* = \sum_{k=1}^q \rho_k \mathbf{u}_k \mathbf{v}_k^* \quad (57)$$

leads to

- spatial (\mathbf{U}) and temporal (\mathbf{V}) EOFs (orthonormal)
- singular values ρ_i (stored on the diagonal of \mathbf{D})

They are also solution of

$$\begin{aligned} \mathbf{X}\mathbf{v} &= \rho\mathbf{u} \\ \mathbf{X}^*\mathbf{u} &= \rho\mathbf{v}, \end{aligned} \Rightarrow \begin{aligned} \mathbf{X}\mathbf{X}^*\mathbf{u} &= \rho^2\mathbf{u} \\ \mathbf{X}^*\mathbf{X}\mathbf{v} &= \rho^2\mathbf{v} \end{aligned} \quad (58)$$

Spatial and temporal modes can be obtained via SVD decomposition!

Properties

- Conventionally (positive) singular values are ordered by decreasing value.
- A given mode j contributes to the explained variance as the squared norm of $\mathbf{u}_j \rho_j \mathbf{v}_j^*$, ie: ρ_j^2 .
- The total variance in the data (squared norm of \mathbf{X}) equals the sum of all squared singular values:

$$\text{trace}(\mathbf{X}\mathbf{X}^*) = \text{trace}(\mathbf{X}^*\mathbf{X}) = \|\mathbf{X}\|_2^2 = \sum_{k=1}^q \rho_k^2, \quad (59)$$

is a measure of the total variance (also sometimes abusively called energy) in the system. The ratio $f_k = \rho_k^2 / \sum_{k=1}^q \rho_k^2$ is thus a measure of the variance contained in mode k compared to the overall energy and one often says that mode k explains $100 f_k$ % of the variance and that the first K modes explain $100 \sum_{k=1}^K \rho_k^2 / \sum_{k=1}^q \rho_k^2$ % of the total variance.

Properties

- The first p modes define thus the best base using p base vectors in which the data can be expressed with minimum loss of information.
- Truncation can be used to filter data by rejecting modes.
- First modes often have physical meaning, the following less (due to orthogonality constraint).
- EOF very efficient for standing patterns, less for propagating features (try to generate synthetic data and look at SVD decomposition).
- Space and time can be interchanged.
- Calculate eigenvalues on smallest covariance matrix, eigenvalues are the same !
- No explicit information on "distance" or "time", only covariances are relevant.
- Data can be reordered without changing the EOFs.
- 2D spatial data can be packed into 1D arrays.

Truncation

$$\mathbf{X}_N = \mathbf{U}_N \mathbf{D}_N \mathbf{V}_N^* = \sum_{k=1}^N \rho_k \mathbf{u}_k \mathbf{v}_k^* \quad (60)$$

is the best approximation to \mathbf{X} using only N spatial modes

The covariance matrix $\mathbf{X}\mathbf{X}^*$ can also be approximated by using the truncated representation of \mathbf{X}

$$\mathbf{X}_N \mathbf{X}_N^* = \mathbf{U}_N \mathbf{D}_N \mathbf{V}_N^* \mathbf{V}_N \mathbf{D}_N^* \mathbf{U}_N^* = \mathbf{U}_N \mathbf{D}_N \mathbf{D}_N^* \mathbf{U}_N^* = \tilde{\mathbf{U}} \tilde{\mathbf{U}}^* \quad (61)$$

where $\tilde{\mathbf{U}}$ is matrix \mathbf{U}_N where each column is multiplied by the associated singular value.

This reduced rank covariance matrix is specially useful in Data Assimilation or Optimal Interpolation

Truncation rejects some data as noise, hence SVD can be used as filtering tool

Generalisations

- Values of the state vector can accommodate complex values, allowing complex EOF on 2D vectors (horizontal velocities, gradients ...), Fourier transforms, Hilbert transforms, etc
- Multivariate EOFs $\mathbf{x}^* = (\mathbf{T}^*, \mathbf{S}^*, \mathbf{p}^*, \dots)$ (needs proper non dimensional form)
- SSA, lagged covariances to detect autocorrelations in time

$$\mathbf{X} = \begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_n \\ x_2 & x_3 & x_4 & \dots & x_1 \\ \dots & \dots & \dots & \dots & \dots \\ x_k & \dots & \dots & \dots & x_{k-1} \end{pmatrix}, \quad (62)$$

- MSSA, temporally lagged spatial fields

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \dots & \mathbf{x}_n \\ \mathbf{x}_2 & \mathbf{x}_3 & \mathbf{x}_4 & \dots & \mathbf{x}_1 \\ \dots & \dots & \dots & \dots & \dots \\ \mathbf{x}_k & \dots & \dots & \dots & \mathbf{x}_{k-1} \end{pmatrix}, \quad (63)$$

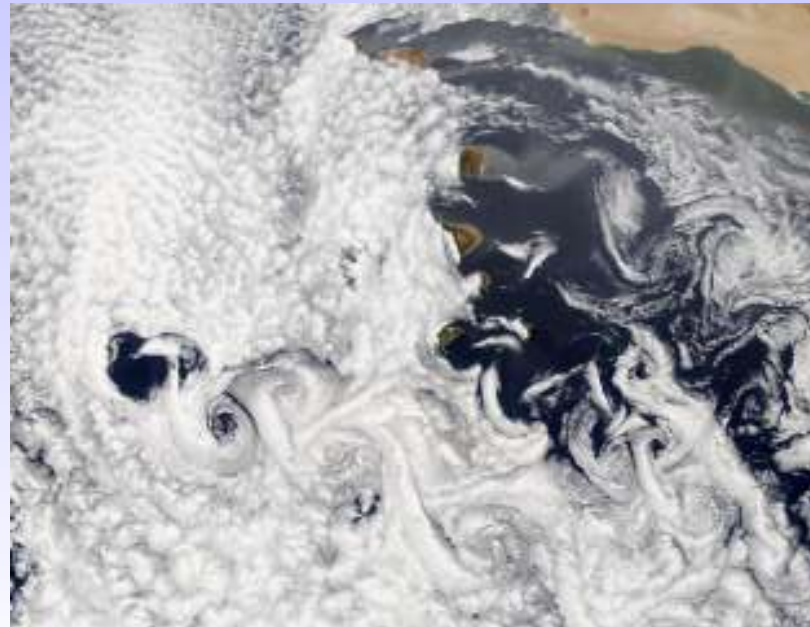
Applications

- Analysis of variability
- Data compression
- Filtering
- Data synthesizing
- Model intercomparison (time-space error distinctions, phase-amplitude error distinctions)
- Objective analysis (or optimal interpolation) of in-situ data: use of vertical EOFs and horizontal objective analysis of their amplitudes to reduces the number of data during the costly optimal interpolation
- Reducing the size of a problem by projecting (complex) reference model equations onto a small number of Principal Components
- Simplify forecasts by using any extrapolation method (neural networks, genetic algorithms etc) on temporal modes
- Ensemble preparation for assimilations
- Calculation of covariances (remember OI ?):

The Problem

EOFs and friends are powerful tools to analyze data and reduce the dimensionality of a problem. However, the decomposition assumes the data matrix \mathbf{X} (or continuous function f) to be known.

Missing data must be imputed before performing EOF analysis



Data *IN*terpolating EOF: *DINEOF* interpolation

- Large scale EOFs should not be influenced by local changes in the values of a few points
- Large scale EOFs can thus be estimated by using a first guess of missing data
- Then, once the larger scale EOFs and their amplitudes are estimated, they can serve to calculate the value of the field at the missing points by

$$(\mathbf{X}_a)_{ij} = (\mathbf{U}_N \mathbf{D}_N \mathbf{V}_N^*)_{ij} = \sum_{k=1}^N \rho_k (\mathbf{u}_k)_i (\mathbf{v}_k^*)_j, \quad (64)$$

- EOFs themselves can be re-evaluated and the process can be repeated until convergence.
- What is the optimal number N of relevant EOFs to be retained to recompose the signal at the missing data points ?

Optimal number N of EOFs: Cross validation technique

- Set aside a random set of valid data (random points or random clouds).
- Use the EOF interpolation and calculate an error estimate based on the rms distance between the interpolated field at these points and the data set aside there
- Start with 1 EOF, fill in, calculate rms error, continue by filling in with a second EOF until convergence, calculate rms error ...
- Provides reconstruction error as a function of number of EOF retained.
- The optimal truncation is the one that minimises the diagnosed error.

Once the optimal number know, perform a last iteration with this number of EOFs reinjecting the data set aside for cross-validation.

DINEOF

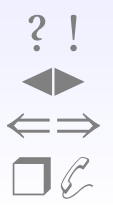
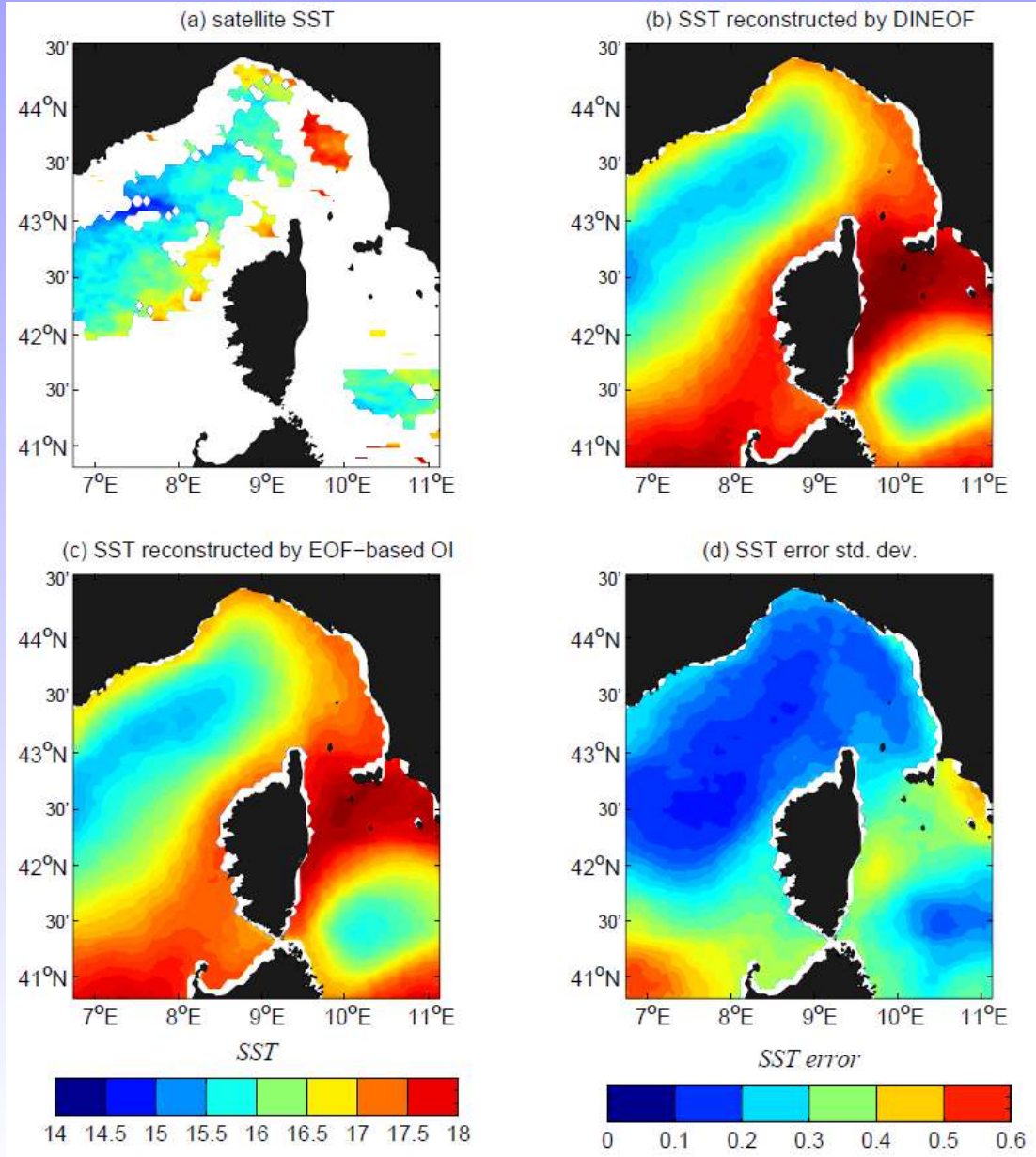
- Implementation much more rapid than OI version.
- Problem: no natural error maps in DINEOFs

Error maps:

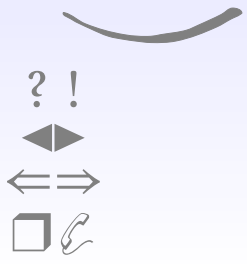
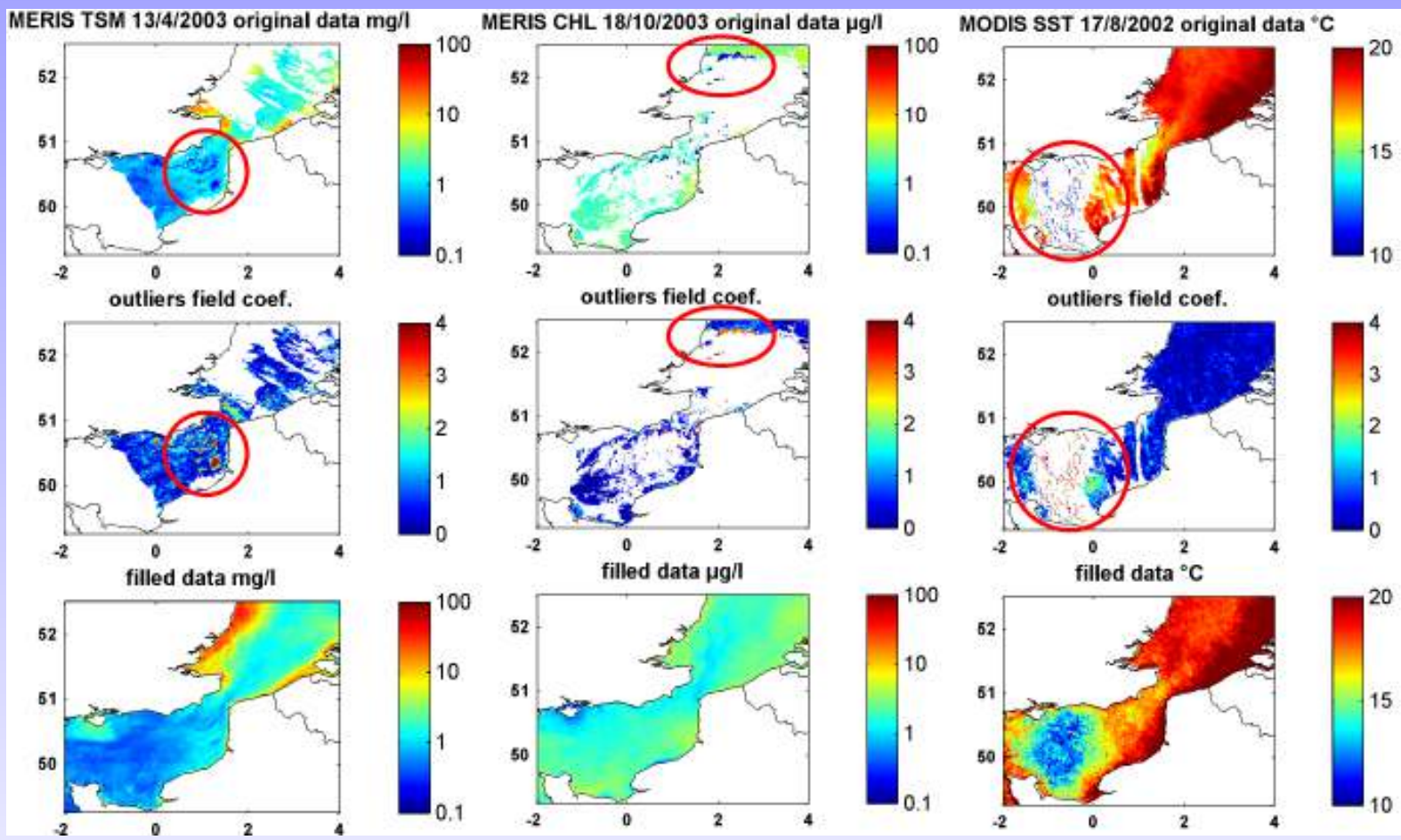
- Use error estimate from OI version (35)
- Numerical verification that difference OI-DINEOF is smaller than this error
- Can also be exploited to detect strange pixels in original data (outlier detection using spatial covariances)

CANNOT see things under clouds which are due to patterns never seen before (EOF are exploiting past pattern)

Error maps

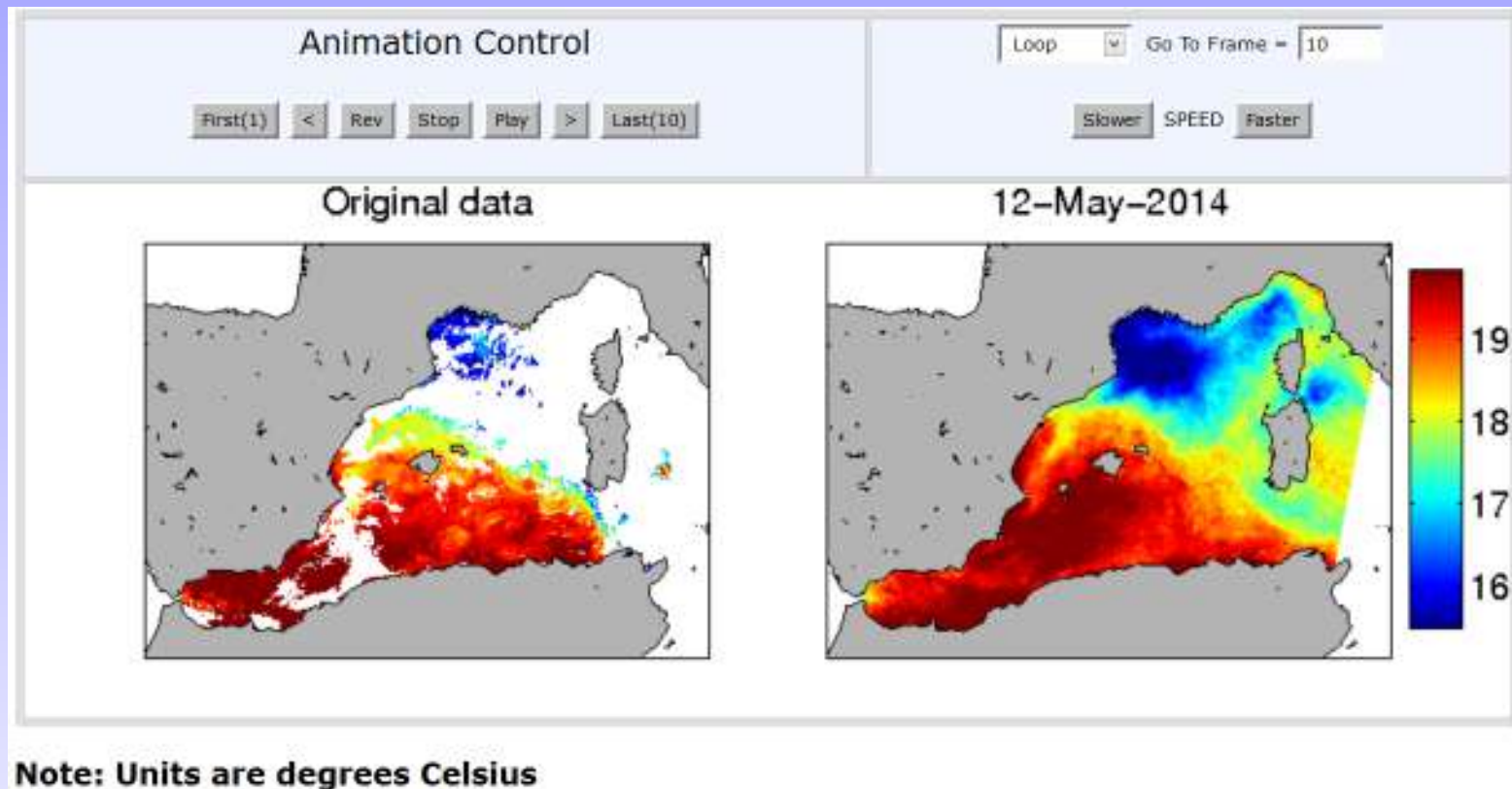


Outlier detection



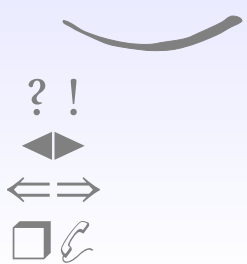
Operational use example

Daily 10 day period based on last six month EOFs



<http://gher-diva.phys.ulg.ac.be/DINEOF/dineof.html>

- *Gridding*
- *DIVA theory*
- *Implementations and exercises*
- *DINEOF theory*
- ***Implementations and exercises***



On line version: beta version



web DINEOF v0.3.5 Not signed in Help Sign in Sign up

Please define all parameters for running DINEOF analysis:

Select dataset:	SEVIRI-V2_MYOCEAN_L3C_EUR	DINEOF processing parameters	
Select variable:	adjusted_sea_surface_temperature [kelvin]	Strength of the filter (alpha)	0.01
Select grid size:	0.05	Number of iterations of the filter (numit)	10
Select region:	Mediterranean Sea - Balearic Islands	Max number of modes (nev)	5
Select filtering:	Please select filtering	Max number of iterations (nitemax)	300
Define filtered out values between; NaN and NaN		Min % of clear data from the whole scene (min_clear)	3.0
Min: [>=]			
Max: [<=]			
Define date range between: 2013-08-12 and 2014-05-17			
Define starting date/time:	2013-08-12		
Define ending date/time:	2013-09-03		
Your email address:	JM.Beckers@ulg.ac.be		

<http://gher-dineof01.phys.ulg.ac.be:8081/>



Make it work

"Parameter free" method, yet some things to decide

- Time and space window for data: neither too small nor too large: Cover the scale you are interested in with several repetitions in time (EOFs!)
- Subtraction of mean field (remember background in OI?): The better your first guess, the better the result
- Number of EOFs to retain a priori for Krylov space before cross validation: small value reduces CPU time but should be larger than final number of EOFs retained
- Reinforce temporal coherence (EOFs do not know explicitly about "distance"): avoid spikes
- How to validate: incorporated cross-validation, additional cross-validation (add clouds on your side), validation with independent (in-situ) data
- Keep original data in unclouded regions or analyzed data: Most coherent approach is to use analyzed field everywhere

Even more decisions

- Number of iterations: neither too few nor too many
- Criteria for convergence: neither too severe nor too relaxed
- Elimination of images or pixels with too few data: threshold typically $\sim 3\%$
- Normalisation in case of multivariate approaches
- Exploitation of delayed information (*eg.* wind a few hours before TSM field)

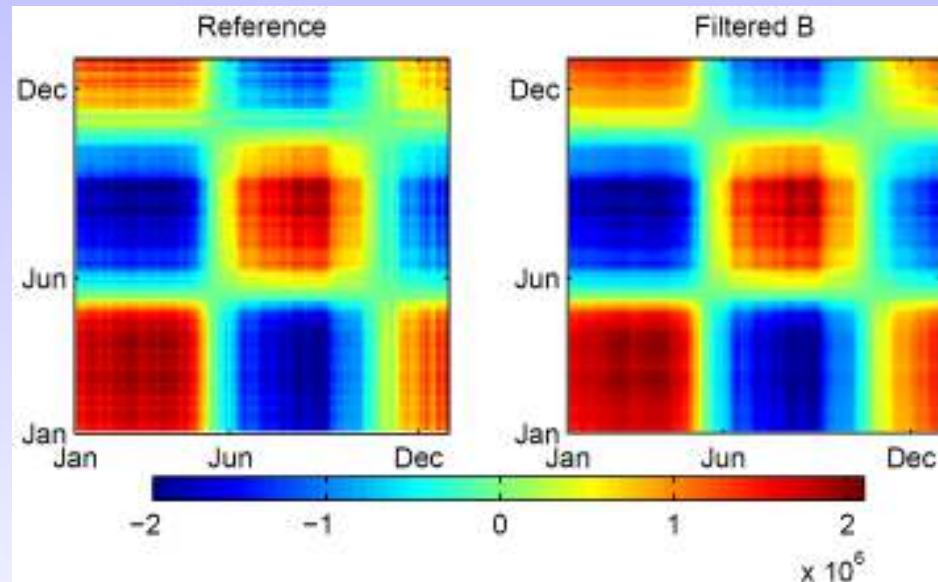
Temporal coherence

Application of time-filtering matrix F to data X would lead to filtered data \tilde{X}

$$\tilde{X} = XF \quad (65)$$

Incorporation into the DINEOF iterations?

Instead of working with covariance X^*X work with filtered covariance matrix (EOFs are the eigenvectors) F^*X^*XF .



Construction of filtering operator F

How to construct filter matrix (operator) F : by mimicking effect of diffusion in space

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} \quad (66)$$

translated into time filtering (diffusion in time direction) as iterations

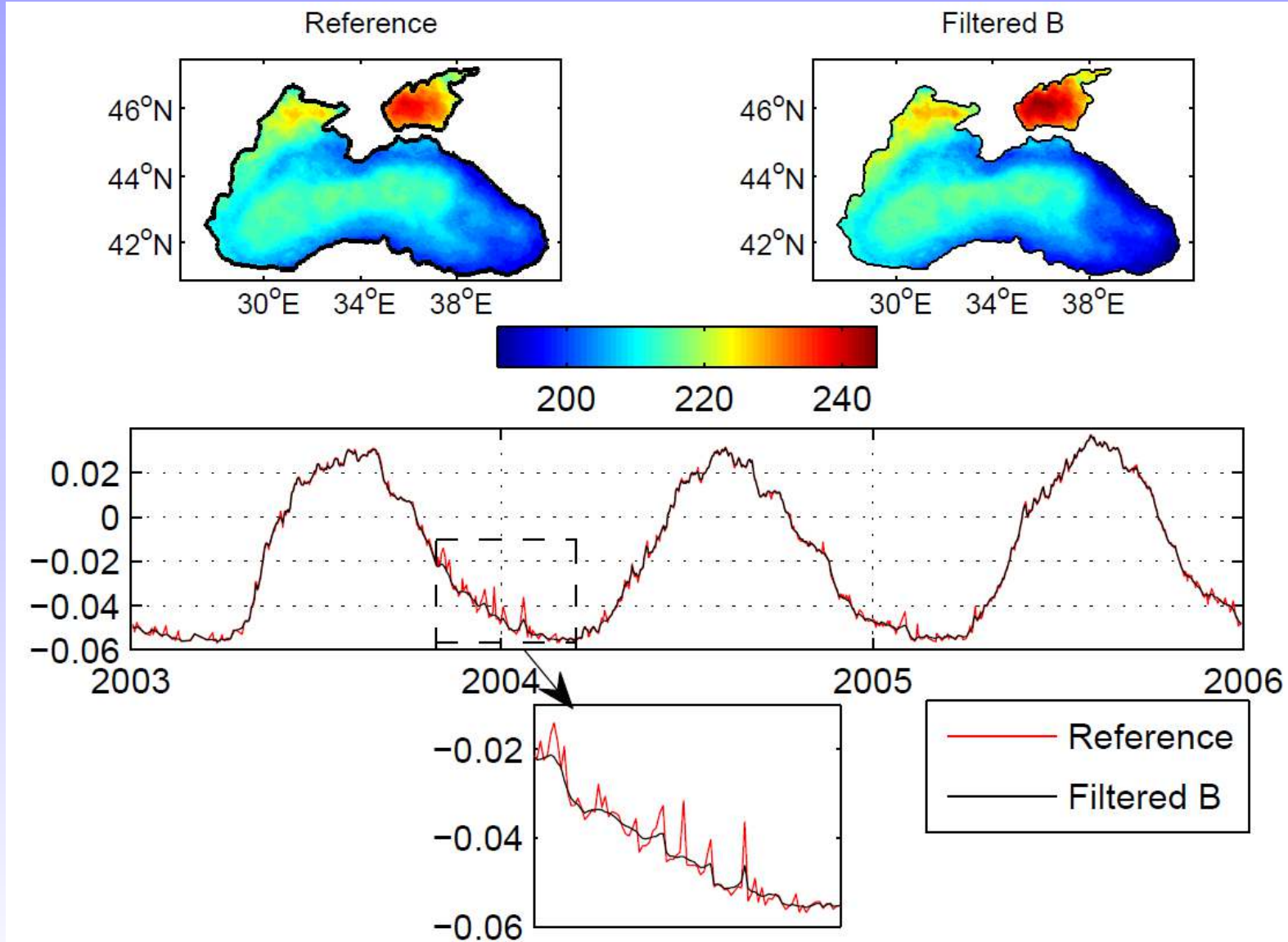
$$\mathbf{x}_i^{(s+1)} = \mathbf{x}_i^{(s)} + \frac{\mathbf{G}_{i+1} - \mathbf{G}_i}{t'_{i+1} - t'_i} \quad (67)$$

$$\mathbf{G}_{i+1} = \alpha \frac{\mathbf{x}_{i+1}^{(s)} - \mathbf{x}_i^{(s)}}{t_{i+1} - t_i} \quad (68)$$

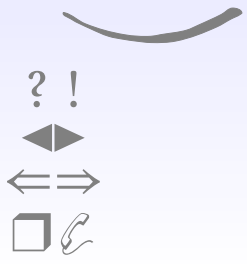
$$t'_i = \frac{t_i + t_{i-1}}{2} \quad (69)$$

with iterations $s = 1, 2, 3, \dots, p$ and strength α of filter defining filter characteristics (*Alvera et al 2009*)

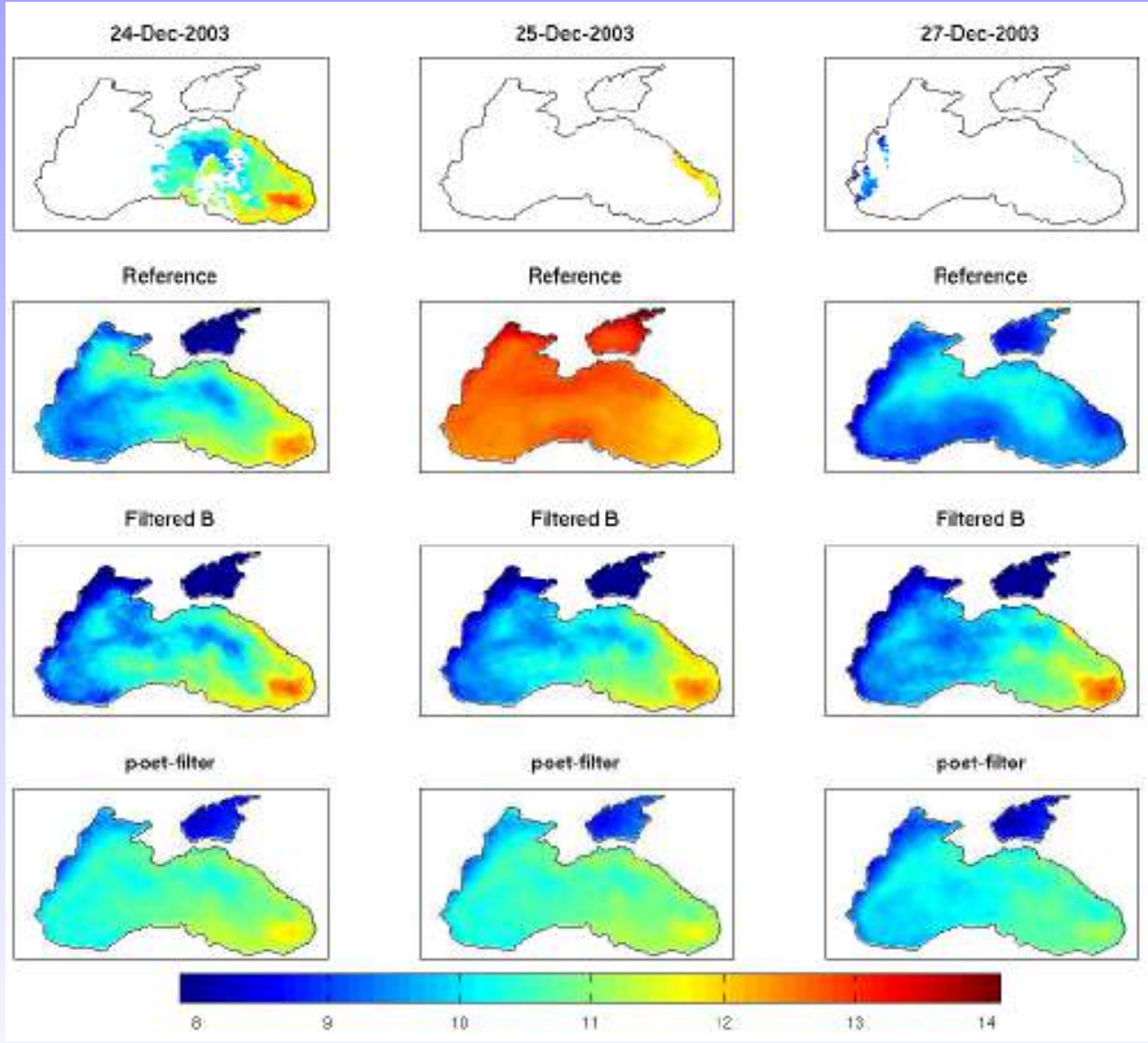
Effect of filtering



Université de Liège

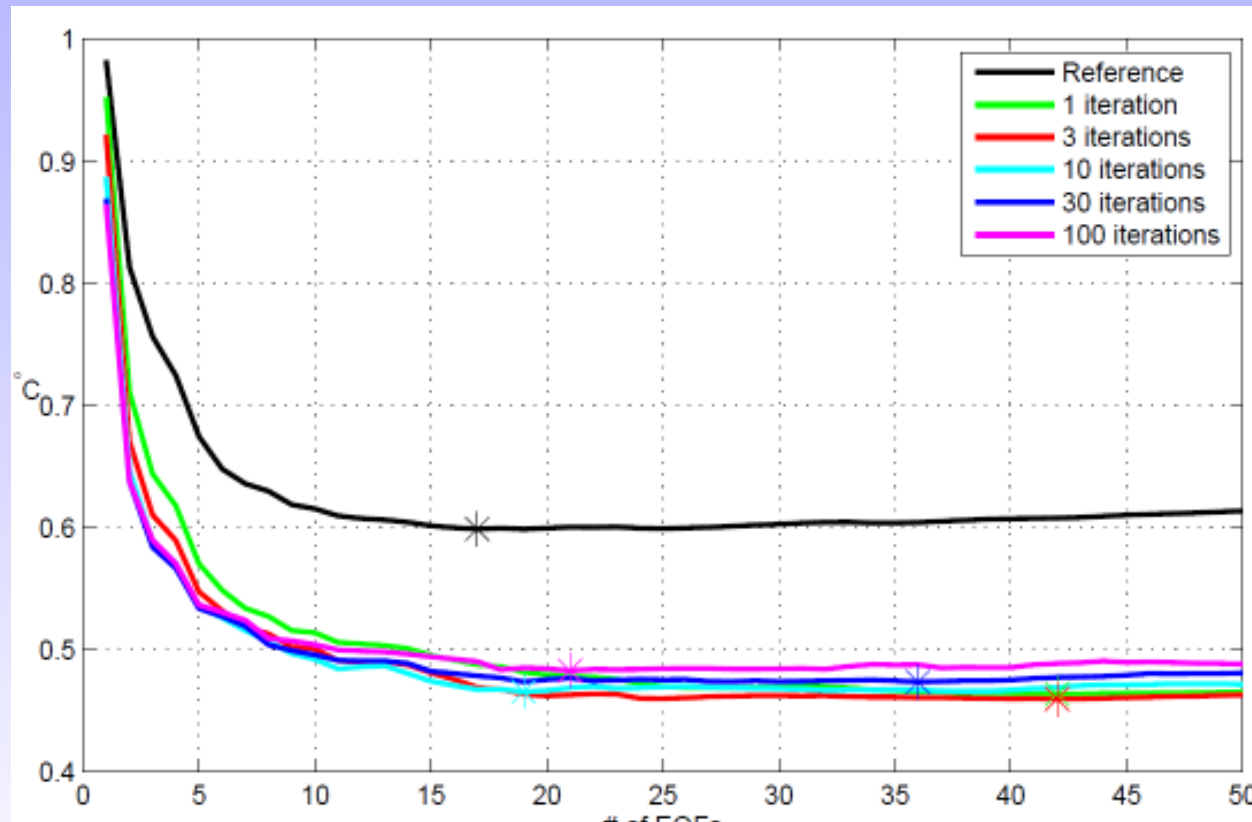


Effect of filtering



How to decide on values for filtering

- Your decision to filter out processes shorter than $T: 2\pi\sqrt{\alpha p} \sim T$ and α such that filtering iterations remain stable $\alpha < \min(\Delta t)^2/2$
- By cross validation again !

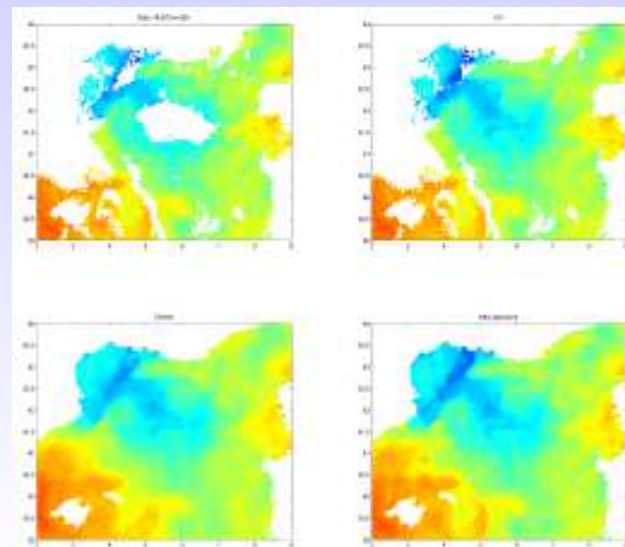



Command line version


<http://modb.oce.ulg.ac.be/mediawiki/index.php/DINEOF>


- DINEOF Fortran code with a lot of matlab/octave tools around.
- Next version with better netCDF support
- Google usergroup
<http://groups.google.com/group/dineof>
- SVN for contributors


In next version: possibility to add small scale OI on top of DINEOF interpolation





 A. Alvera-Azcárate, D. Sirjacobs, A. Barth, and J.-M. Beckers. Outlier detection in satellite data using spatial coherence. *Remote Sensing of Environment*, 119:84-91, 2012.


 D. Sirjacobs, A. Alvera-Azcárate, A. Barth, G. Lacroix, Y. Park, B. Nechad, K. Ruddick, J.-M. Beckers. Cloud filling of ocean color and sea surface temperature remote sensing products over the Southern North Sea by the Data Interpolating Empirical Orthogonal Functions methodology. *Journal of Sea Research*, 65(1):114-130. 2011.

 A. Alvera-Azcárate, A. Barth, D. Sirjacobs, J.-M. Beckers. Enhancing temporal correlations in EOF expansions for the reconstruction of missing data using DINEOF. *Ocean Science*, 5, 475-485, 2009

 A. Alvera-Azcárate, A. Barth, J.-M. Beckers, and R. H. Weisberg. Multivariate reconstruction of missing data in sea surface temperature, chlorophyll and wind satellite fields. *Journal of Geophysical Research*, 112:C03008, 2007.
doi:10.1029/2006JC003660.

 J.-M. Beckers, A. Barth, and A. Alvera-Azcarate. DINEOF reconstruction of clouded images including error maps. Application to the Sea Surface Temperature around Corsican Island. *Ocean Science*, 2(2):183-199, 2006.

 A. Alvera-Azcárate, A. Barth, M. Rixen, and J.-M. Beckers. Reconstruction of incomplete oceanographic data sets using Empirical Orthogonal Functions. Application to the Adriatic Sea. *Ocean Modelling*, 9:325-346, 2005.

 J.-M. Beckers and M. Rixen. EOF calculations and data filling from incomplete oceanographic data sets. *Journal of Atmospheric and Oceanic Technology*, 20(12):1839-1856, 2003

