Generating balanced fields in Kalman Filtering

ESA Summer school 2010

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? !

Outline

- ***Kalman Filter***
- ***Ensemble Kalman Filter***
- ***Balanced initialisation***
- ***Balanced perturbations***
- ***Parameter estimation***

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- ***Kalman Filter***
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Remember Optimal Interpolation

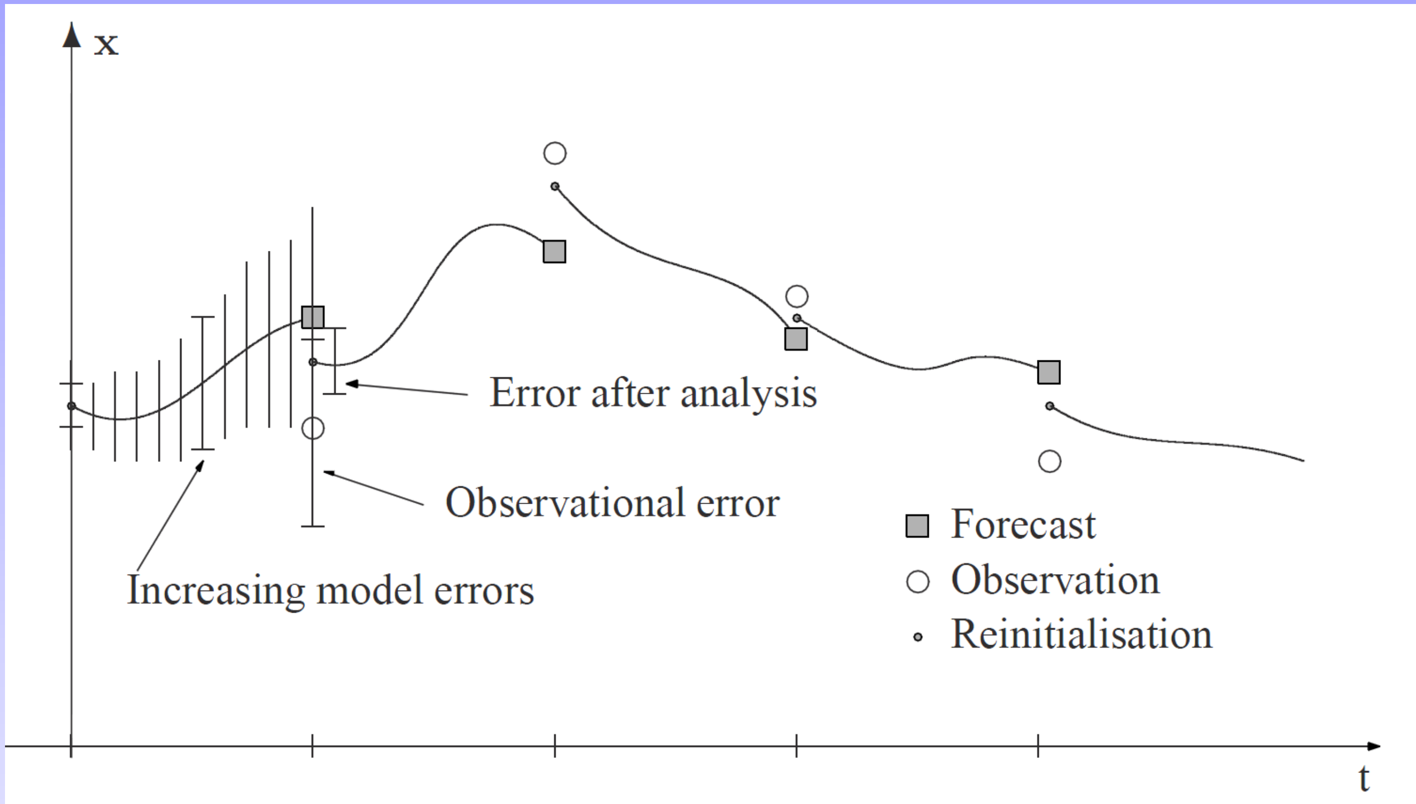
$\mathbf{y}$ is a very large vector grouping all P observation including eg, satellite images and the state vector $\mathbf{x}$ is an even larger vector of M model results,

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{P}^f \mathbf{H}^{\mathrm{T}} \left(\mathbf{H}\mathbf{P}^f \mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1} \left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right), \quad (1)$$

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\,\mathbf{P}^f = \left(\mathbf{I} - \mathbf{P}^f \mathbf{H}^{\mathrm{T}} \left(\mathbf{H}\mathbf{P}^f \mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1} \mathbf{H}\right) \mathbf{P}^f. \quad (2)$$

When repeated intermittently: control of time evolution.

Extended Kalman Filter



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Where is the model involved ?

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{P}^f\mathbf{H}^{\mathrm{T}}\left(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right). \tag{3}$$

Where is the model involved ?

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{P}^f\mathbf{H}^\mathrm{T}\left(\mathbf{H}\mathbf{P}^f\mathbf{H}^\mathrm{T} + \mathbf{R}\right)^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right). \qquad (4)$$

- $\mathbf{x}^f$ updated by the model
- $\mathbf{P}^f$! At the very least it was updated at previous assimilation cycle but in reality errors a advected, diffused ...

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The model

$$\mathbf{x}_{n+1} = \boldsymbol{\mathcal{M}}(\mathbf{x}_n) + \boldsymbol{f}_n + \boldsymbol{\eta}_n \tag{5}$$

where $\boldsymbol{\eta}_n$ takes into account errors introduced by the model and $\boldsymbol{f}_n$ includes the external forcings. n is the assimilation cycle stepping, not the (much finer) model time stepping.
Linearization for error analysis:

$$\mathbf{x}^f_{n+1} = \mathbf{M}\,\mathbf{x}^a_n + \boldsymbol{f}_n + \boldsymbol{\eta}_n \tag{6}$$

The true state evolves without modeling errors and obeys

$$\mathbf{x}^t_{n+1} = \mathbf{M}\,\mathbf{x}^t_n + \boldsymbol{f}_n \tag{7}$$

so that the forecast error $\boldsymbol{\epsilon}^f = \mathbf{x}^f - \mathbf{x}^t$ satisfies

$$\boldsymbol{\epsilon}^f_{n+1} = \mathbf{M}\,\boldsymbol{\epsilon}^a_n + \boldsymbol{\eta}_n. \tag{8}$$

Multiplying this equation by its transposed version to the right and using the statistical average we get the so-called Lyapunov equation, which allows the advancement in time of the error-covariance matrix:

Error evolution

$$\mathbf{P}^f_{n+1} = \mathbf{M}\mathbf{P}^a_n\mathbf{M}^{\mathrm{T}} + \mathbf{Q}_n = \mathbf{M}(\mathbf{M}\mathbf{P}^a_n)^{\mathrm{T}} + \mathbf{Q}_n \quad (9)$$

with the definition of the model-error covariance matrix

$$\mathbf{Q}_n = \left\langle \boldsymbol{\eta}_n \boldsymbol{\eta}_n^{\mathrm{T}} \right\rangle . \quad (10)$$

Error covariance can be advanced in time starting from known error on initial condition

$$\mathbf{P}_0 = \left\langle (\mathbf{x}_0 - \mathbf{x}_0^t)(\mathbf{x}_0 - \mathbf{x}_0^t)^{\mathrm{T}} \right\rangle . \quad (11)$$

Kalman filter

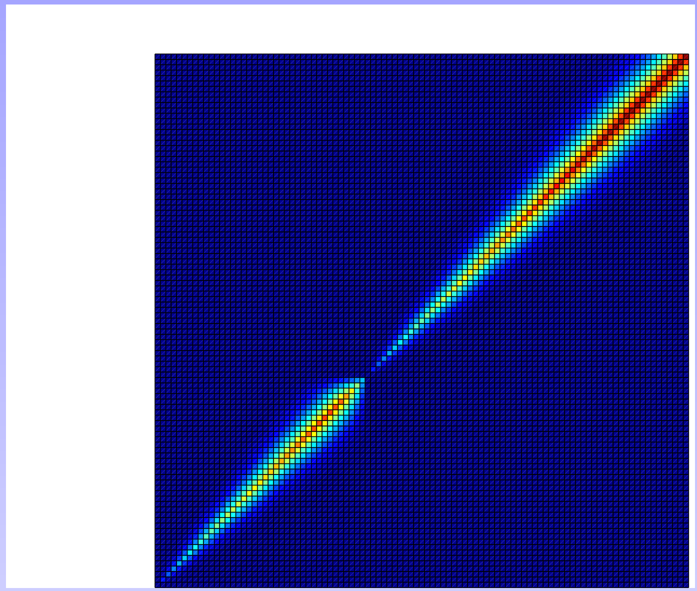
Initialisation:
$$\begin{aligned}\mathbf{x}_0^a &= \mathbf{x}^i \\ \mathbf{P}_0^a &= \mathbf{P}^i\end{aligned}$$

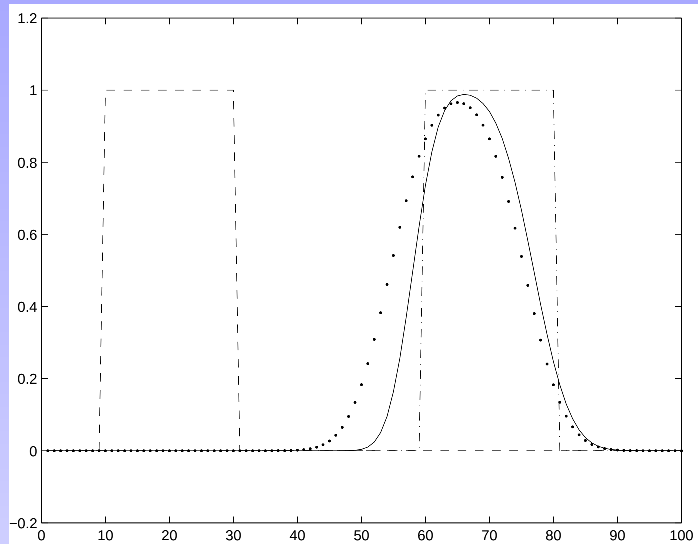
Forecast:
$$\begin{aligned}\mathbf{x}_{n+1}^f &= \boldsymbol{\mathcal{M}}(\mathbf{x}_n^a) + \boldsymbol{f}_n \\ \mathbf{P}_{n+1}^f &= \mathbf{M}_n \mathbf{P}_n^a \mathbf{M}_n^T + \mathbf{Q}_n\end{aligned}$$

Analysis:
$$\begin{aligned}\mathbf{K}_{n+1} &= \mathbf{P}_{n+1}^f \mathbf{H}_{n+1}^T \left(\mathbf{H}_{n+1}\mathbf{P}_{n+1}^f \mathbf{H}_{n+1}^T + \mathbf{R}_{n+1}\right)^{-1} \\ \mathbf{x}_{n+1}^a &= \mathbf{x}_{n+1}^f + \mathbf{K}_{n+1}\left(\mathbf{y}_{n+1} - \mathbf{H}_{n+1}\mathbf{x}_{n+1}^f\right) \\ \mathbf{P}_{n+1}^a &= \mathbf{P}_{n+1}^f - \mathbf{K}_{n+1}\mathbf{H}_{n+1}\mathbf{P}_{n+1}^f\end{aligned}$$

Note nonlinear model and linear error propagation

Toy example





1D advection with numerical diffusion and incorrect advection. A fixed "observation system" is placed at node 40. Note the error covariance increase downstream (left panel) and the model results improvment (right panel).

Some slight problems

With a model of M unknowns (10^7) and P observations (10^6)

- Size of **P**: M^2, unable to store
- Cost of updating **P**: M model runs instead of 1, unable to calculate
- Inversion of $\left(\mathbf{H}\mathbf{P}^f\mathbf{H}^\mathrm{T} + \mathbf{R}\right)$: P^3: unable to calculate
- Appearance of M^T: adjoint model, tricky to program and unique to each model

Are we stuck to toy problems ? Or to downgrade the filter ?

- fixed $\mathbf{P}^f$: optimal interpolation
- fixed and diagonal $\mathbf{P}^f$ and $\mathbf{R}$: nudging (equivalent to relaxation term in equations $-(x-y)/T$)
- fixed and diagonal $\mathbf{P}^f$ with zero $\mathbf{R}$: direct insertion

The more we simplify the more prone the filter will be to inconsistencies, sometimes downgrading results instead of improving.

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One solution, Reduced-rank Kalman Filter

IF we can write

$$\mathbf{P} \sim \mathbf{S}\mathbf{S}^{\mathrm{T}} \tag{12}$$

where **S** is of size $M \times K$, $K \ll M$, then

- storage of **S** instead of **P** (cost of K model instances)
- a matrix multiplication by **P** (M^3) is replaced by two successive multiplications involving **S** ($2KM^2$)

If we assume a diagonal $\mathbf{R} = \mu^2 \mathbf{I}$, the matrix inversion cost in the analysis step is reduced from P^3 to K^3:

$$\mathbf{P}\mathbf{H}^{\mathrm{T}} \left(\mathbf{H}\mathbf{S}\mathbf{S}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right)^{-1} = \mathbf{S}\mathbf{U}^{\mathrm{T}} \left(\mathbf{U}\mathbf{U}^{\mathrm{T}} + \mu^2 \mathbf{I}\right)^{-1} = \mathbf{S} \left(\mathbf{U}^{\mathrm{T}}\mathbf{U} + \mu^2 \mathbf{I}\right)^{-1} \mathbf{U}^{\mathrm{T}}. \tag{13}$$

again Sherman-Morisson at work with $\mathbf{U} = \mathbf{H}\mathbf{S}$ of dimension $P \times K$ with $K \ll P$

Effect of reduced rank?

Analysis step expressed in terms of **S**

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{S}\boldsymbol{\alpha}, \quad \boldsymbol{\alpha} = \left(\mathbf{U}^{\mathrm{T}}\mathbf{U} + \mu^2\mathbf{I}\right)^{-1}\mathbf{U}^{\mathrm{T}}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right). \qquad (14)$$

where $\boldsymbol{\alpha}$ is a $K \times 1$ vector: the increment is only in a space spanned by the K columns of **S**. Error propagation remains also within this space.
How to choose this space ? Remember EOFs ? Create **S** from EOFs of model runs for example.

- *Kalman Filter*
- ***Ensemble Kalman Filter***
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Creating S

Instead of creating several model runs to calculate EOFs, directly apply statistics on different model runs ! Create K model runs by perturbing parameters (initial conditions, forcings, parameters, topography...) and calculate

$$\bar{\mathbf{x}} = \frac{1}{K} \sum_{j=1}^{K} \mathbf{x}^{(j)}. \tag{15}$$

If we accept this as the best estimation of the true state, deviations from this state can be used to estimate the error-covariance matrix

$$\mathbf{P} = \frac{1}{K-1} \sum_{j=1}^{K} \left(\mathbf{x}^{(j)} - \bar{\mathbf{x}}\right) \left(\mathbf{x}^{(j)} - \bar{\mathbf{x}}\right)^{\mathrm{T}}. \tag{16}$$

The columns of **S** are directly given by the ensemble members, shifted to have a zero mean and scaled by $1/\sqrt{K-1}$.
However: convergence of variance estimations from K samplings converges only as $1/\sqrt{K}$: large ensemble or create ensemble with optimal distributions of its members (Evensen 2004).

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How to generate perturbations or initial conditions

Too brutal perturbations will generate unrealistic model evolutions with unrealistic high frequency motions excited. If increment creates too much noise, filter increment !

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{F}\mathbf{P}^f\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^f\mathbf{H}^T + \mathbf{R}\right)^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^f\right). \quad (17)$$

But how to design the filter **F** ?

Example of gravity waves

In a flat bottom shallow water system, elevation η and transports U, V satisfy volume conservation and momentum:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial U}{\partial x} - \frac{\partial V}{\partial y} \tag{18}$$

$$\frac{\partial U}{\partial t} = fV - gh\frac{\partial \eta}{\partial x} \tag{19}$$

$$\frac{\partial V}{\partial t} = -fU - gh\frac{\partial \eta}{\partial y} \tag{20}$$

Inadequate initialization will trigger Poincaré waves which will not dissipate without strong friction. Fourier analysis

$$\tilde{\eta}(k_x, k_y, \omega) = \int_3 \eta(x, y, t) e^{-i(k_x x + k_y y - \omega t)} dx dy dt \tag{21}$$

Poincare modes

$$-i\omega\tilde{\eta} = -ik_x\tilde{U} - ik_y\tilde{V} \quad (22)$$

$$-i\omega\tilde{U} = f\tilde{V} - ighk_x\tilde{\eta} \quad (23)$$

$$-i\omega\tilde{V} = -f\tilde{U} - ighk_y\tilde{\eta} \quad (24)$$

$$\omega \begin{pmatrix} \tilde{\eta} \\ \tilde{U} \\ \tilde{V} \end{pmatrix} = \begin{pmatrix} 0 & k_x & k_y \\ ghk_x & 0 & if \\ ghk_y & -if & 0 \end{pmatrix} \begin{pmatrix} \tilde{\eta} \\ \tilde{U} \\ \tilde{V} \end{pmatrix} = \mathbf{M} \begin{pmatrix} \tilde{\eta} \\ \tilde{U} \\ \tilde{V} \end{pmatrix} \quad (25)$$

$$\mathbf{M} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1} \quad (26)$$

Modes

$\mathbf{M} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1}$ where $\mathbf{D}$ is a diagonal matrix, with the following elements:

$$\omega_0 = 0 \quad (27)$$

$$\omega_1 = s \quad (28)$$

$$\omega_2 = -s \quad (29)$$

and $s = \sqrt{f^2 + ghk_x^2 + ghk_y^2}$. The first solution represents the geostrophic equilibrium and the second and third solutions are inertia-gravity waves, also called Poincaré waves. The corresponding eigenvectors are the columns of the $\mathbf{V}$ matrix:

$$\mathbf{V} = \begin{pmatrix} 1 & 1 & 1 \\ -\frac{ighk_y}{f} & \frac{k_x s + ifk_y}{k_x^2 + k_y^2} & -\frac{k_x s - ifk_y}{k_x^2 + k_y^2} \\ \frac{ighk_x}{f} & \frac{k_y s - ifk_x}{k_x^2 + k_y^2} & -\frac{k_y s + ifk_x}{k_x^2 + k_y^2} \end{pmatrix} \quad (30)$$

Getting rid of Poincare modes in Fourier space

The filtered quantities are denoted by a prime.

$$\begin{pmatrix} \tilde{\eta}' \\ \tilde{U}' \\ \tilde{V}' \end{pmatrix} = \mathbf{V} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \mathbf{V}^{-1} \begin{pmatrix} \tilde{\eta} \\ \tilde{U} \\ \tilde{V} \end{pmatrix} \tag{31}$$

(read the formular from the right). Perfoming the matrix multiplications yieds

$$\mathbf{F} = \frac{1}{f^2 + ghk_x^2 + ghk_y^2} \begin{pmatrix} f^2 & ifk_y & -ifk_x \\ -ighfk_y & ghk_y^2 & -ghk_xk_y \\ ighfk_x & -ghk_xk_y & ghk_x^2 \end{pmatrix}. \tag{32}$$

It is sufficient to filter first the elevation $\tilde{\eta}'$,

$$\tilde{\eta}' = \frac{f^2\tilde{\eta} + ifk_y\tilde{U} - ifk_x\tilde{V}}{f^2 + ghk_x^2 + ghk_y^2}, \tag{33}$$

? !

Filter in Fourier space

Use

$$\tilde{\eta}' = \frac{f^2\tilde{\eta} + ifk_y\tilde{U} - ifk_x\tilde{V}}{f^2 + ghk_x^2 + ghk_y^2}, \qquad (34)$$

and then compute the filtered transport by the following equations:

$$\tilde{U}' = -\frac{ighk_y}{f}\tilde{\eta}' \qquad (35)$$

$$\tilde{V}' = \frac{ighk_x}{f}\tilde{\eta}' \qquad (36)$$

In real space ?

Filter not very practical since in Fourier space.

$$\left(f^2 + ghk_x^2 + ghk_y^2\right)\tilde{\eta}' = f^2\tilde{\eta} + ifk_y\tilde{U} - ifk_x\tilde{V} \qquad (37)$$

If the inverse Fourier transform is applied to the previous equation, one obtains a differential equation which the filtered solution must satisfy:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \frac{f^2}{gh}\right)\eta' = \frac{1}{h}\frac{\partial V}{\partial x} - \frac{1}{h}\frac{\partial U}{\partial y} - \frac{f^2}{gh}\eta \qquad (38)$$

On the right-hand side of equation (38), the potential vorticity of the flow (linearized by assuming that $|\eta| \ll h$ and that the relative vorticity is much smaller than the planetary vorticity) can be recognized. The inverse Fourier transform applied to equations (35) and (36) gives the geostrophic equilibrium.

$$U' = -\frac{gh}{f}\frac{\partial \eta'}{\partial y} \qquad V' = \frac{gh}{f}\frac{\partial \eta'}{\partial x} \qquad (39)$$

Filter in practise

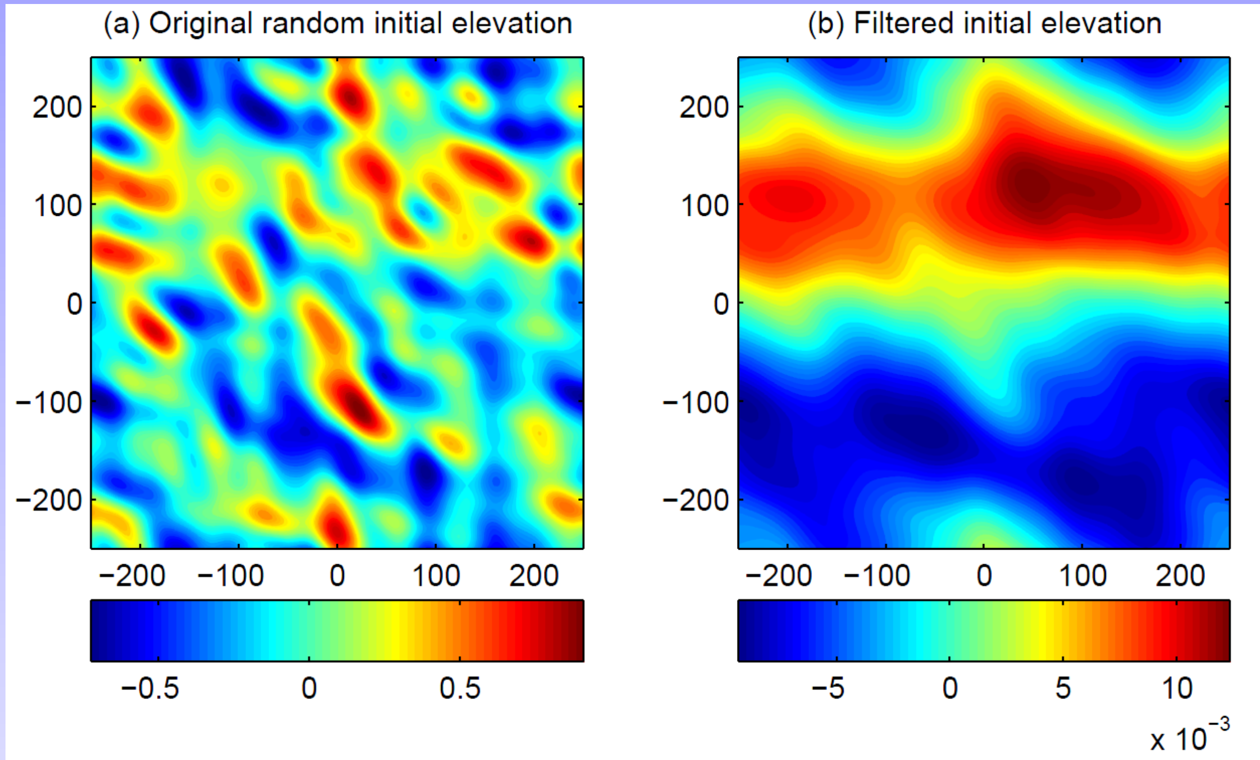
Filter= calculate increment to define rhs of (38), then solve (38) to find filtered η' from which to deduce filtered transports. Generalization to variable h via interpretation in terms of potential vorticity on the rhs.

$$\frac{\partial^2 \eta'}{\partial y^2} + \frac{\partial^2 \eta'}{\partial x^2} - \frac{f^2}{gh}\eta' = \frac{fq}{g} \tag{40}$$

The initial potential vorticity q is computed from the unfiltered elevation and velocity by:

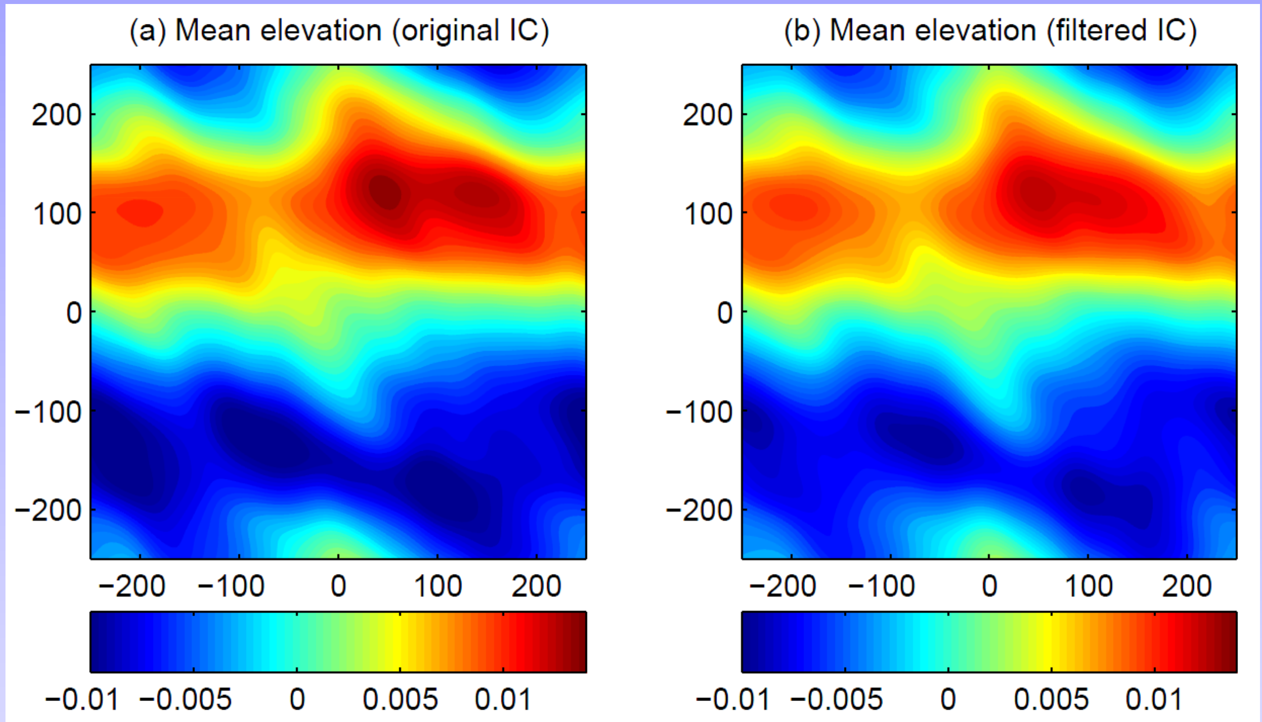
$$q = \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} - \frac{f}{h}\eta \tag{41}$$

Initial condition



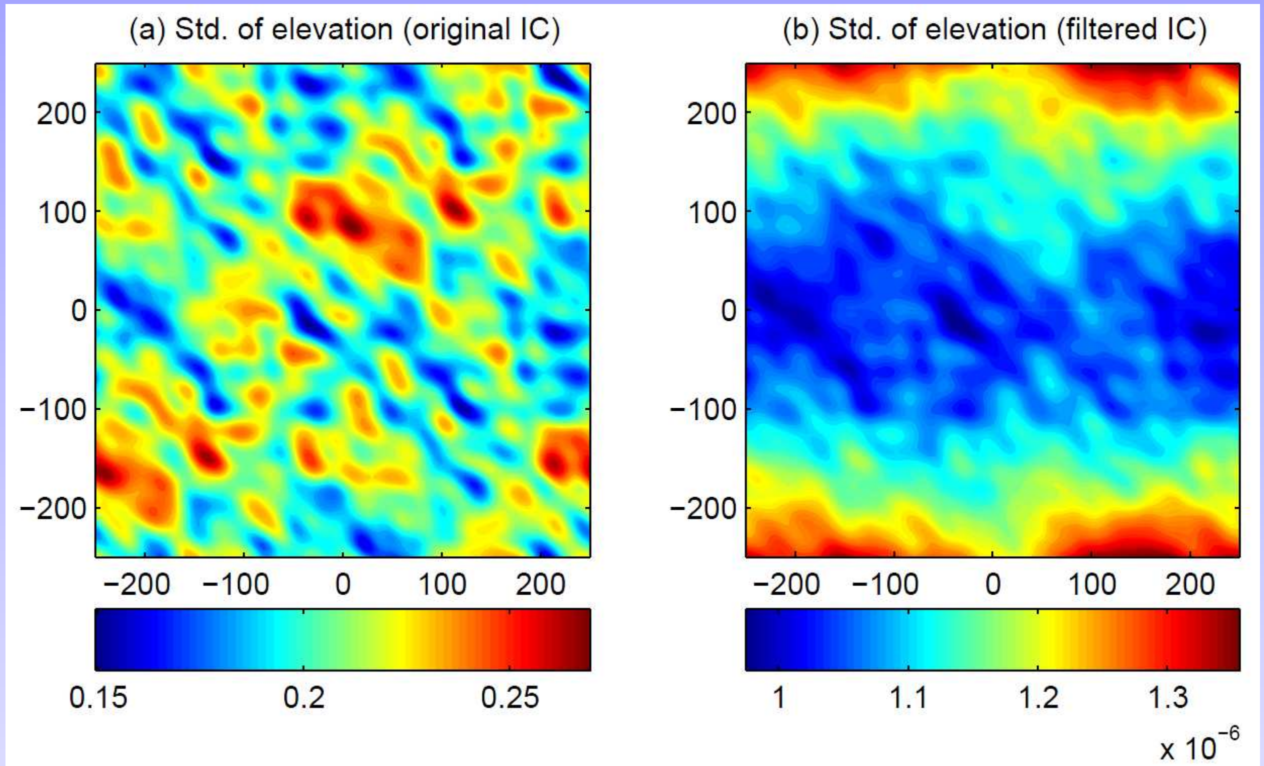
Unfiltered IC and filtered IC

Initial condition



Time average with unfiltered IC and filtered IC

Initial condition



Standart deviation over time with unfiltered IC and filtered IC

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- *Kalman Filter*
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- *Parameter estimation*

Generating perturbations

In open domains, using perturbed Fourier modes leads to perturbations who on average have covariance with Gaussian decrease over a prescribed length scale (Evensen 2002).

Limited to periodic domains and unique length scale. If applied to ocean, problems at coasts.

Generating perturbations via a functional

$$2J = \mathbf{x}^{\mathrm{T}}\mathbf{M}^{\mathrm{T}}\mathbf{W}_M\mathbf{M}\mathbf{x} + \mathbf{x}^{\mathrm{T}}\mathbf{D}^{\mathrm{T}}\mathbf{W}_D\mathbf{D}\mathbf{x} + \mathbf{x}^{\mathrm{T}}\mathbf{W}_E\mathbf{x} \quad (42)$$

- $\mathbf{x}$ will be a perturbation (around zero)
- **W** are weighting matrices (penalizing more or less one term)
- **D** is a spatial derivative operator (as in DIVA), penalizing strong variations
- **M** allows to weakly enforce a constraint (eg. geostrophic equilibrium): $\mathbf{M}\mathbf{x} \sim 0$.

Functional

$$2J = \mathbf{x}^{\mathrm{T}} \mathbf{B}^{-1} \mathbf{x} \tag{43}$$

$$\mathbf{B}^{-1} = \mathbf{M}^{\mathrm{T}} \mathbf{W}_M \mathbf{M} + \mathbf{D}^{\mathrm{T}} \mathbf{W}_D \mathbf{D} + \mathbf{W}_E \tag{44}$$

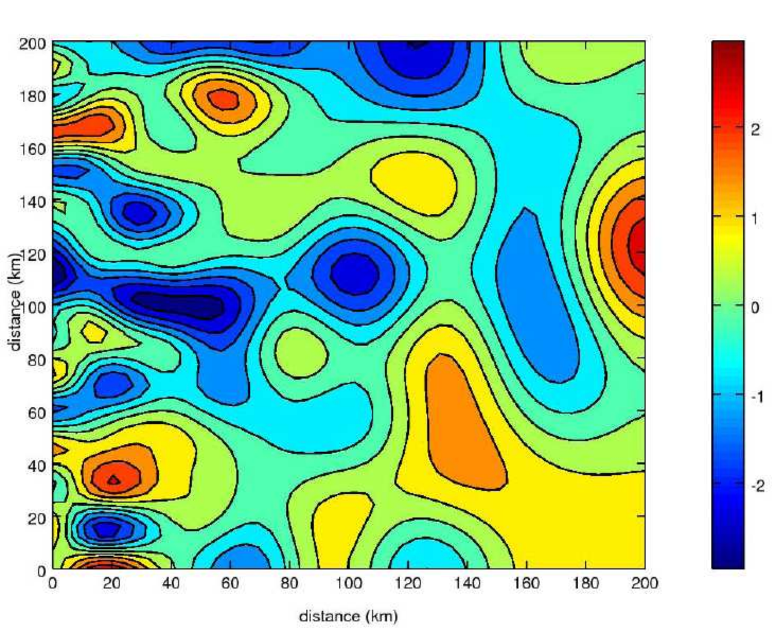
Obviously we are not going to minimize J.
J measure how likely a perturbuation should be: large values of J correspond to unlikely perturbations (not satisfying constraints, lot of variability), while perturbations with low J are welcome.

> Generate a series of perturbation whose probability is proportional to $\exp(-J)$

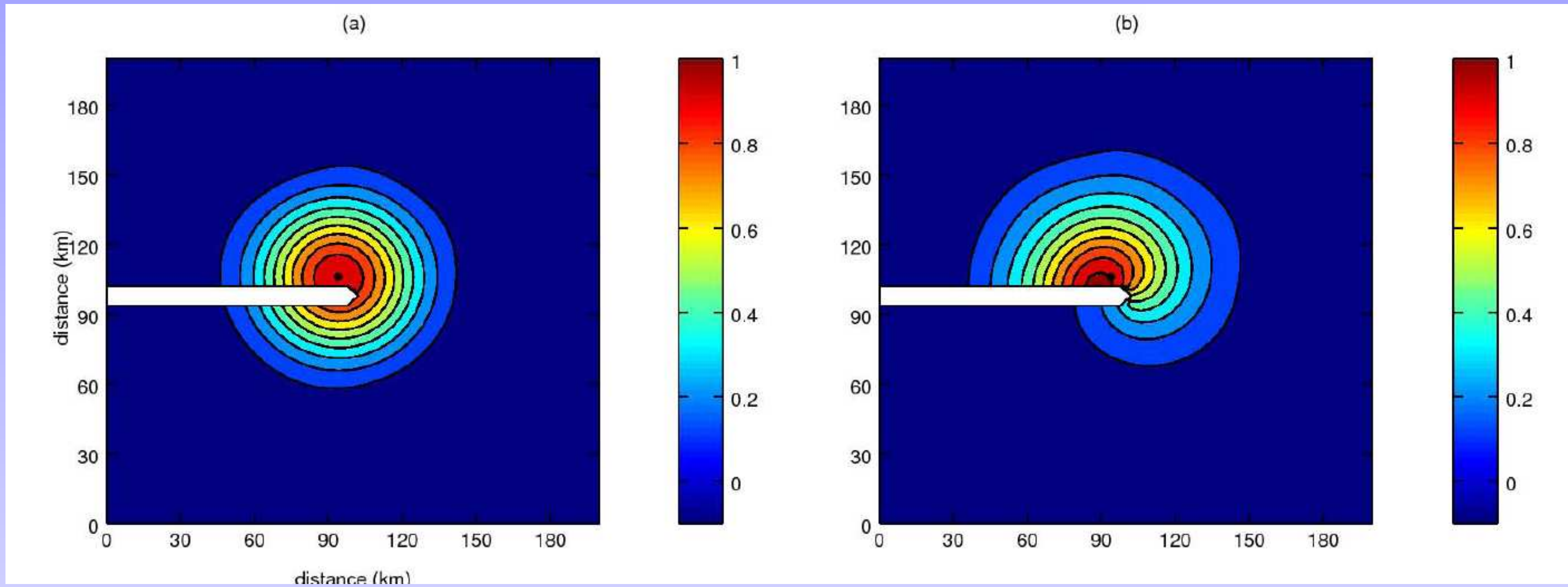
In practice, **D** and **M** are discrete operators which can be translated into sparse matrices. For details, via decomposition of $\mathbf{B}^{-1}$ see papers in the folder.

Example of realisation with variable L

Without weak constraint but with regularity operator changing its intensity in space($\mathbf{W}_D$ is diagonal with different values depending on the location): creation of perturbation having different scales in different regions



Example



Without weak constraint but with regularity operator implemented with "boundary conditions" $\mathbf{n}^{\mathrm{T}}\mathbf{D}\mathbf{x} = 0$. Here wnot a member is shown but from the generated ensemble members we can estimate covariances. Here for a point near the center with all other points. Left: classical generation via Fourier modes, right: generation via constraint version.

Tidally acceptable perturbations

$$\frac{\partial \eta}{\partial t} = -\frac{\partial U}{\partial x} - \frac{\partial V}{\partial y} \quad (45)$$

$$\frac{\partial U}{\partial t} = fV - gh\frac{\partial \eta}{\partial x} \quad (46)$$

$$\frac{\partial V}{\partial t} = -fU - gh\frac{\partial \eta}{\partial y} \quad (47)$$

Tidal motion with given frequency ω with $\eta = \eta'(x,y)e^{i\omega t}$

$$i\omega\eta' = -\frac{\partial U'}{\partial x} - \frac{\partial V'}{\partial y} \quad (48)$$

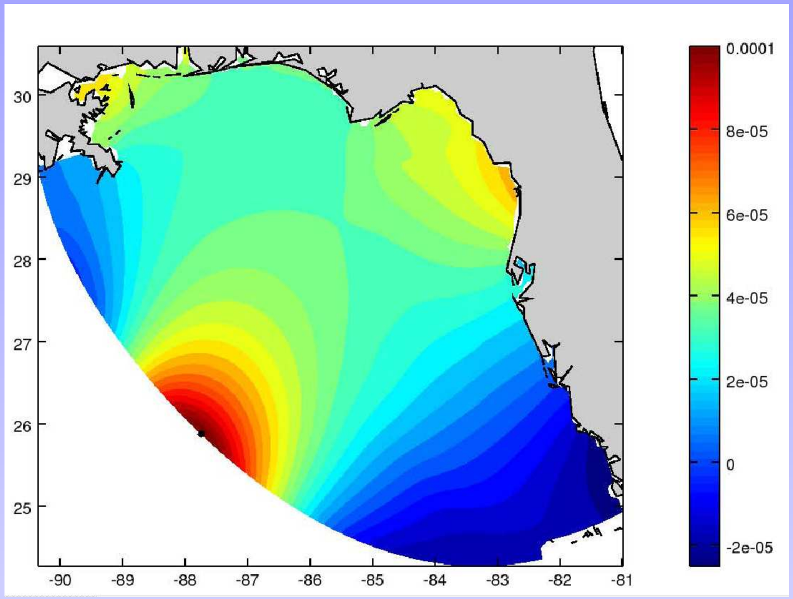
$$i\omega U' = fV' - gh\frac{\partial \eta'}{\partial x} \quad (49)$$

$$i\omega V' = -fU' - gh\frac{\partial \eta'}{\partial y} \quad (50)$$

Can be expressed by sparse matrix operations (finite differences) as

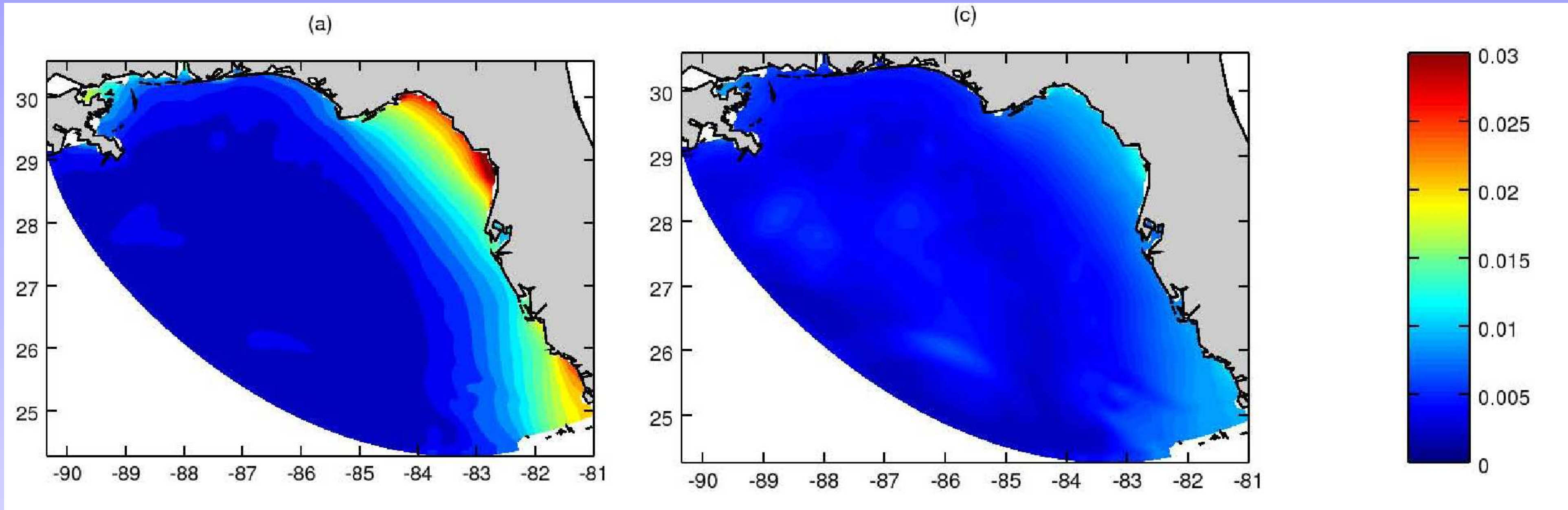
$$\mathbf{Mx} = 0 \quad (51)$$

Example, west Florida coast



Covariance of the point in black with all other points using perturbuations which must weakly satisfy tidal equations. Note the remote correlation !

Example



Unphysical motions with standard perturbations and balanced perturbations

- *Kalman Filter*
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- ***Parameter estimation***

Parameter optimisation

Unorthodox approach:

- Parameter (like wind forcing) = state variable
- Model= observing operator

With ensemble run of perturbed state (parameter), apply Kalman filter extension using ensemble members (k)

$$(\mathbf{S})_k = \frac{1}{\sqrt{N-1}} \left(\mathbf{x}^{(k)} - \langle \mathbf{x} \rangle \right) \tag{52}$$

$$(\mathbf{E})_k = \frac{1}{\sqrt{N-1}} \left(h\left(\mathbf{x}^{(k)}\right) - \langle h\left(\mathbf{x}\right) \rangle \right) \tag{53}$$

$$\mathbf{S}\mathbf{E}^{\mathrm{T}} = \mathrm{cov}(\mathbf{x}^b, h(\mathbf{x}^b)) \tag{54}$$

$$\mathbf{E}\mathbf{E}^{\mathrm{T}} = \mathrm{cov}(h(\mathbf{x}^b), h(\mathbf{x}^b)) \tag{55}$$

Estimation

Kalman fitler approach for a better estimate of forcing field having observed variables in your domain (question normally solved with inverse approaches using adjoints)

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{S}\mathbf{E}^{\mathrm{T}} \left(\mathbf{E}\mathbf{E}^{\mathrm{T}} + \mathbf{R}\right)^{-1} \left(\mathbf{y} - h(\mathbf{x}^b)\right) \tag{56}$$

Now you know how to make this expression manageable ?

Estimation

Kalman fitler approach for a better estimate of forcing field having observed variables in your domain (question normally solved with inverse approaches using adjoints)

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{S}\mathbf{E}^{\mathrm{T}} \left(\mathbf{E}\mathbf{E}^{\mathrm{T}} + \mathbf{R}\right)^{-1} \left(\mathbf{y} - h(\mathbf{x}^b)\right) \tag{57}$$

Now you know how to make this expression manageable ?
Question for the exam next week!

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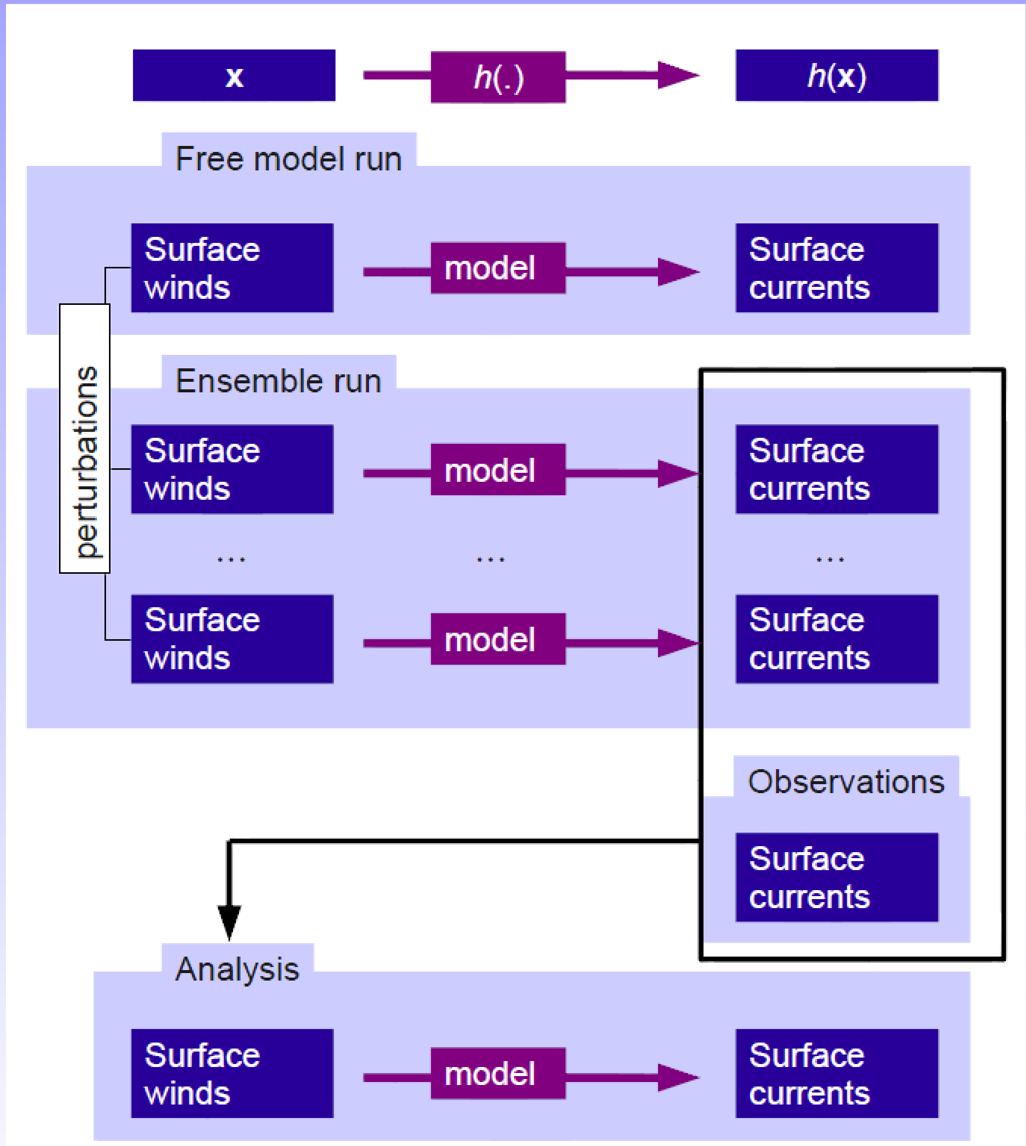
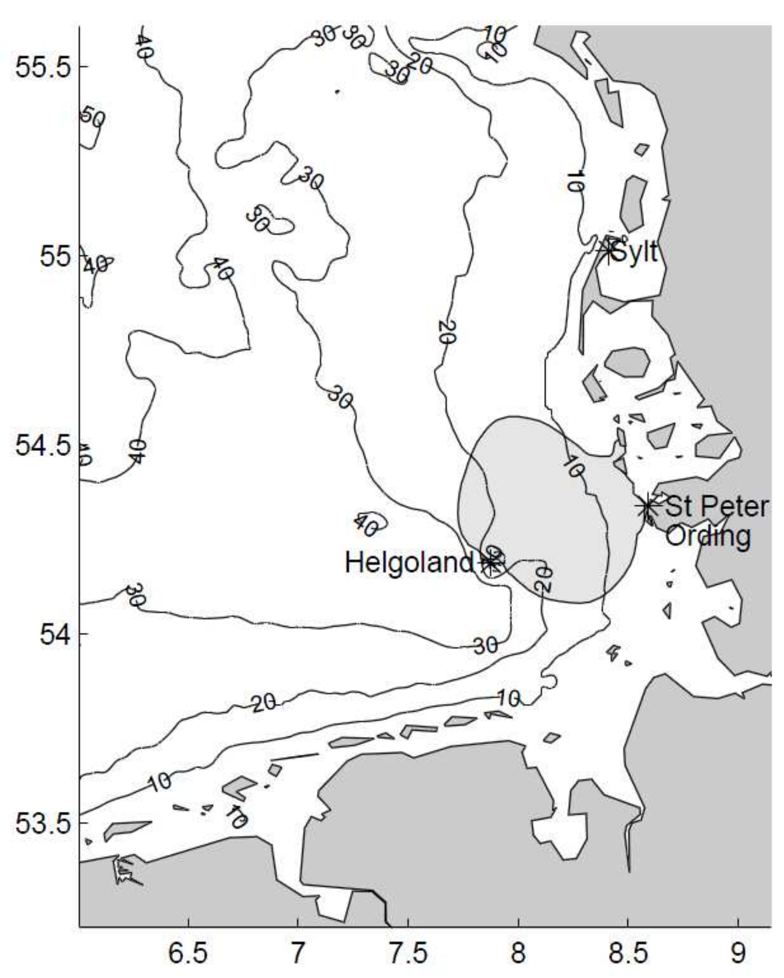
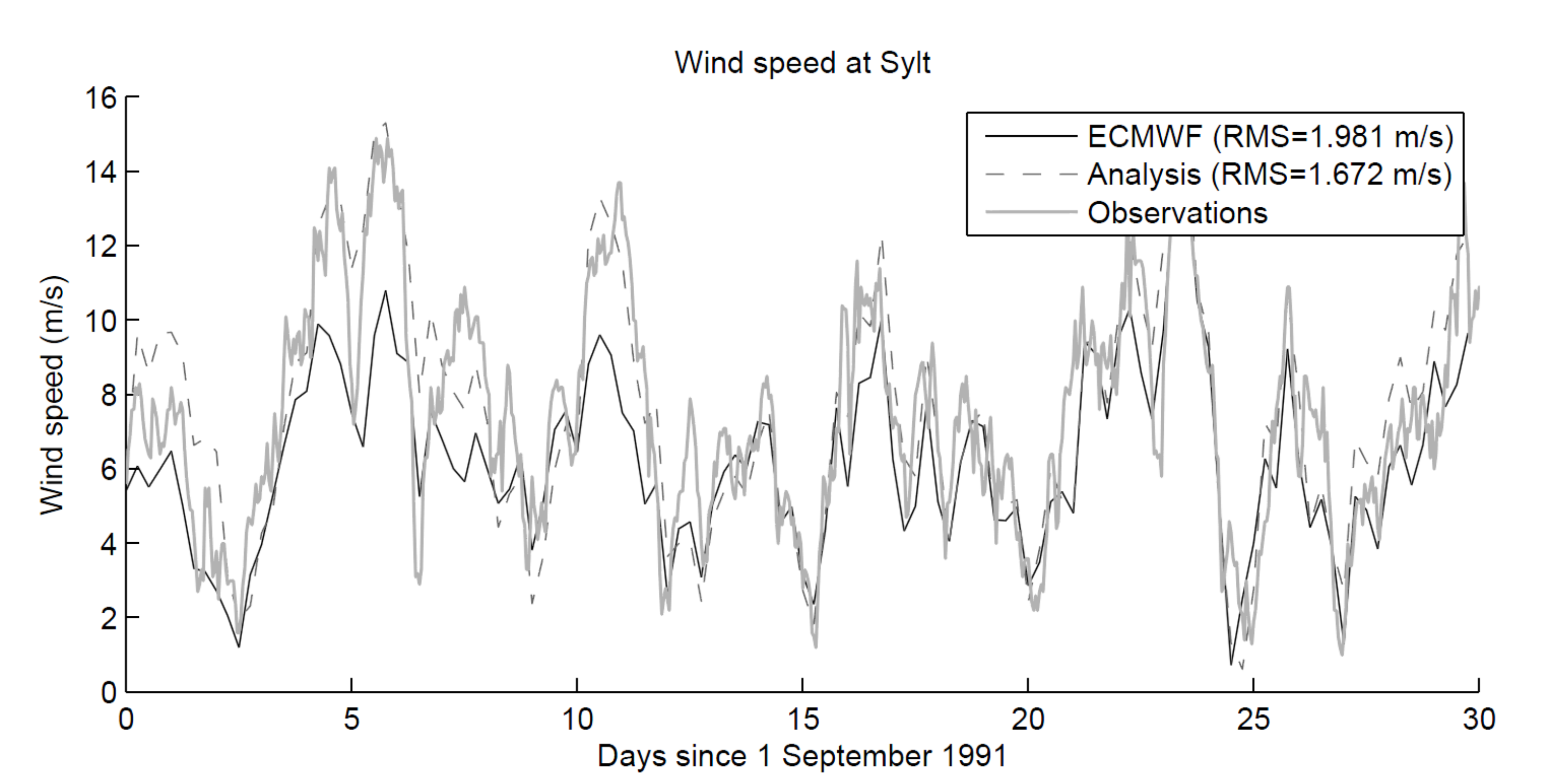
Schematically



Example



Wind field



Improved by assimilating current radar data, without adjoint model

Summary

- Kalman filtering with necessary simplifications
- Ensemble approach
- Problem of balances

Questions ? More details in .pdf files