Localization for Ensemble Kalman Filters - Basics and Recent Results

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Cosmo General Meeting

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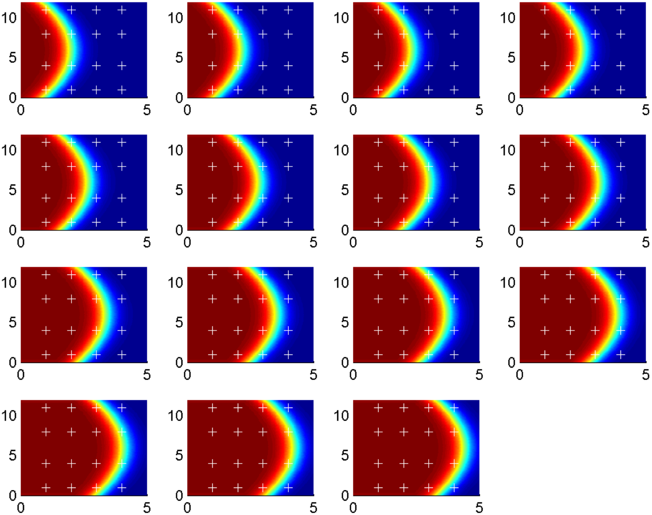
Example 1: Original Dynamics and Measurement Points



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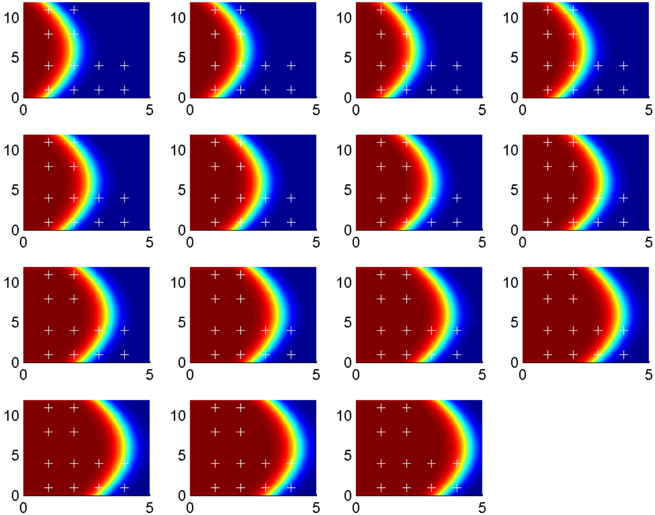

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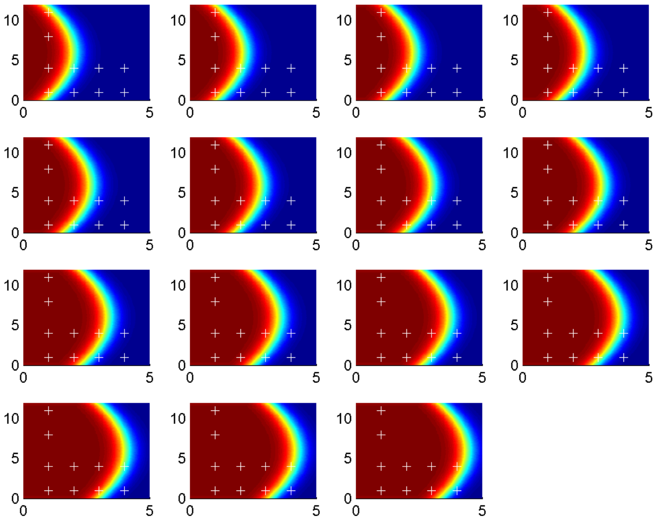

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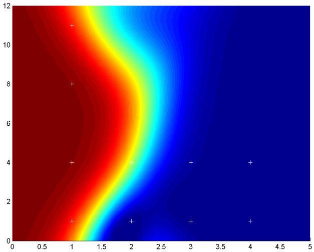

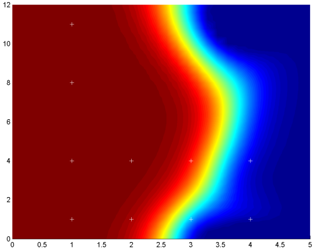

1) Setup a simple example system with a travelling "quadratic" front

2) Dynamics is a shift operator to the right Dynamics is called $M : \varphi_k \mapsto \varphi_{k+1}$

3) Measurement points indicated by white "+", either widely distributed or with some measurement free area

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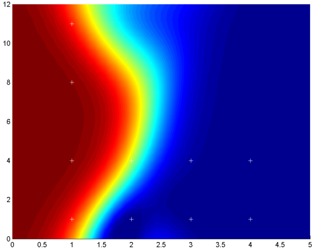

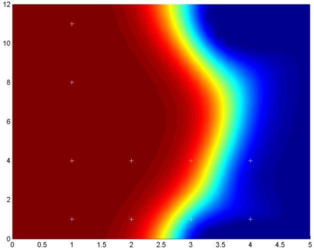

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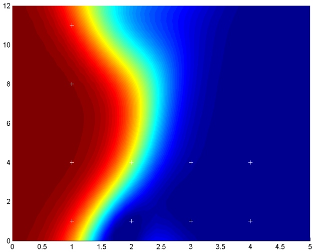

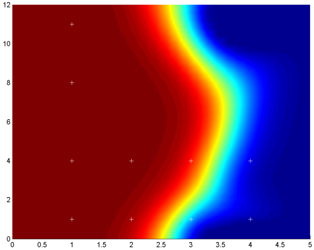

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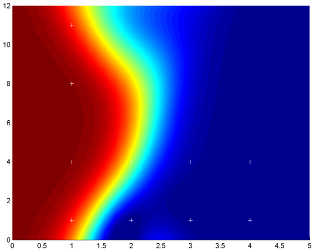

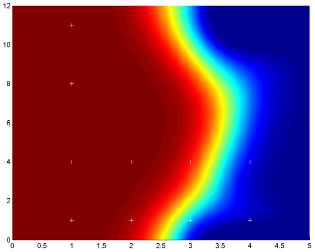

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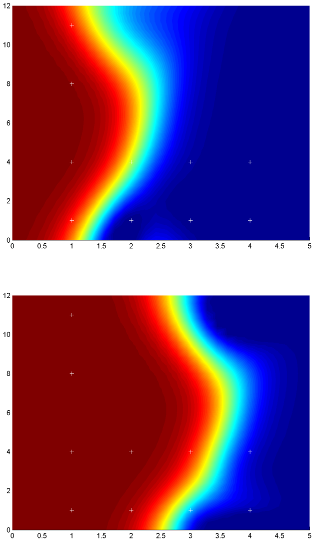

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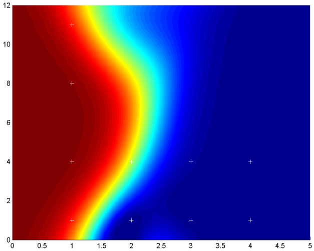

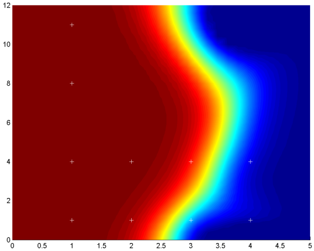

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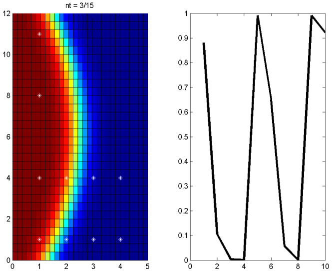
Discretization, Dynamics and Measurement Operator



4) Vectors φ or φ_k at time t_k in $X = \mathbb{R}^N$ describe the field values in a regular grid.

5) Measurement Operator H selects the measurements, next neighbor interpolation.

6) Measurement vector f, time dependence: f_k at time t_k

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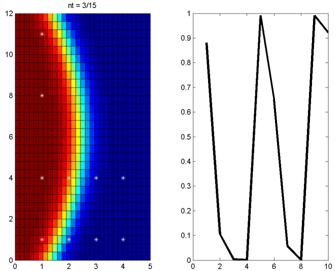

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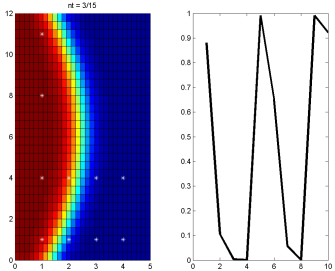

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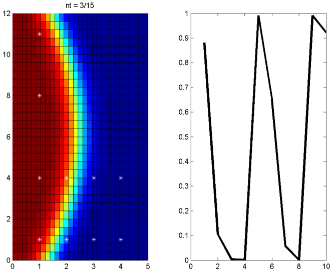

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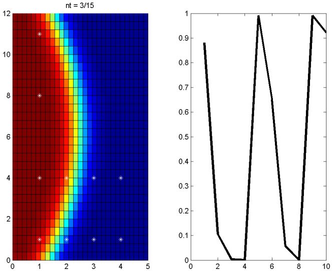

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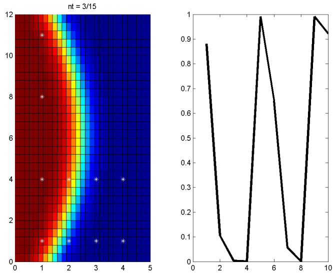

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Outline

Tikhonov Regularization and 3dVar

Kalman Filter: Update B

Ensemble Kalman Filter (EnKF) and Local Ensemble Kalman Filter (LEnKF)

Examples for 3dVar, EnKF and LETKF

Basic Approach

Let H be the data operator mapping the state φ onto the measurements f. Then we need to find φ by solving the equation

$$H\varphi = f \tag{1}$$

When we have some initial guess $\varphi^{(b)}$, we transform the equation into

$$H(\varphi - \varphi^{(b)}) = f - H\varphi^{(b)} \tag{2}$$

with the incremental form

$$\varphi = \varphi^{(b)} + H^{-1}(f - H\varphi^{(b)}). \tag{3}$$

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Regularization 1

Consider an equation

$$H\varphi = f \tag{4}$$

where H^{-1} is unstable or unbounded.

$$\begin{aligned} & H\varphi = f \\ \Rightarrow \quad & H^* H\varphi = H^* f \\ \Rightarrow \quad & (\alpha I + H^* H)\varphi = H^* f. \end{aligned} \tag{5}$$

where $(\alpha I + H^* H)$ has a stable inverse!

Tikhonov Regularization: Replace H^{-1} by the stable version

$$R_\alpha := (\alpha I + H^* H)^{-1} H^* \tag{6}$$

with regularization parameter $\alpha > 0$.

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Regularization 2: Least Squares

Tikhonov regularization is equivalent to the minimization of

$$J(\varphi) := \left(\alpha\|\varphi\|^2 + \|H\varphi - f\|^2\right) \tag{7}$$

The **normal equations** are obtained from *first order optimality conditions*

$$\nabla_\varphi J \stackrel{!}{=} 0. \tag{8}$$

Differentiation leads to

$$\begin{aligned} & 0 = 2\alpha\varphi + 2H^*(H\varphi - f) \\ \Rightarrow \quad & 0 = (\alpha I + H^*H)\varphi - H^*f, \end{aligned} \tag{9}$$

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Covariances and Weighted Norms

Usually, the relation between variables at different points is incorporated by using **covariances / weighted norms**:

$$J(x) := \left(\|\varphi - \varphi^{(b)}\|^2_{B^{-1}} + \|H\varphi - f\|^2_{R^{-1}} \right) \tag{10}$$

The **update formula** is now

$$\varphi = \varphi^{(b)} + (B^{-1} + H^* R^{-1} H)^{-1} H^* R^{-1} (f - H\varphi^{(b)}) \tag{11}$$

or

$$\varphi = \varphi^{(b)} + BH^*(R + HBH^*)^{-1}(f - H\varphi^{(b)}). \tag{12}$$

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How to Update B in KF

Kalman Update Formula for the covariance matrix B (with R error covariance matrix)

$$(B_{k+1}^{(a)})^{-1} = (B_{k+1}^{(b)})^{-1} + H^* R^{-1} H, \quad k = 1, 2, \ldots \tag{13}$$

and for the mean

$$\varphi_{k+1}^{(a)} = \varphi_k^{(b)} + B_{k+1}^{(b)} H^* (H B_{k+1}^{(b)} H^* + R)^{-1} (f_{k+1} - H \varphi_k^{(b)}) \tag{14}$$

for $k = 1, 2, \ldots$ with $B_{k+1}^{(b)}$ being the propagated covariance matrix from $B_k^{(a)}$.

Theorem

For linear systems and linear observation operators 4dVar and the Kalman Filter are equivalent.

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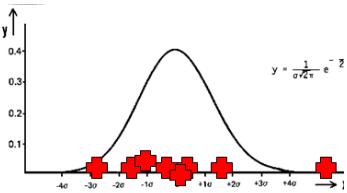
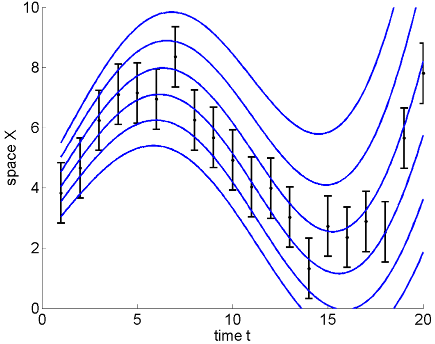
EnKF: *B* via Ensemble of states





Use stochastic estimator

$$B = \mathbb{E}\left\{(\varphi - \overline{\varphi})(\varphi - \overline{\varphi})^T\right\} \tag{15}$$

EnKF Analysis 1

- Updates are

$$\varphi_k = \varphi_k^{(b)} + BH^*\big(R + HBH^*\big)^{-1}\big(f_k - H\varphi_k^{(b)}\big)$$

- The stochastic estimator is given by

$$Q_k = \Big(\varphi^{(1)} - \overline{\varphi}, \ldots, \varphi^{(L)} - \overline{\varphi}\Big), \qquad B = \frac{1}{L-1} Q_k Q_k^T \tag{16}$$

- We solve the 3dVar update in the low-dimensional subspace

$$X_k^{(L)} := \mathrm{span}\Big\{\varphi^{(1)} - \overline{\varphi}, \ldots, \varphi^{(L)} - \overline{\varphi}\Big\} \tag{17}$$

by

$$\varphi_k = \varphi_k^{(b)} + Q_k \underbrace{Q_k^* H^*\big(R + HQ_kQ_k^*H^*\big)^{-1}}_{\text{regularized projection}}\big(f_k - H\varphi_k^{(b)}\big)$$

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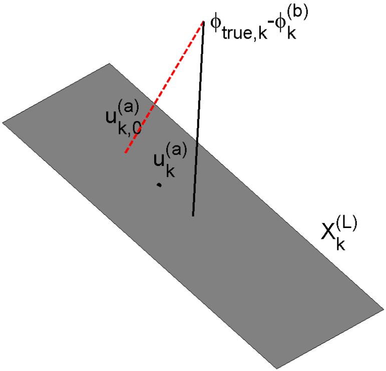

The minimizer of the data term only

$$u_{k,0}^{(a)} = P_k(\varphi_{true,k} - \varphi_k^{(b)})$$

is given by an orthogonal projection.

The minimizer $u_k^{(a)}$ in $X_k^{(L)}$ of

$$J(u) = \|u\|^2_{B^{-1}} + \|(f_k - H\varphi_k^{(b)}) - Hu\|^2_{R^{-1}}$$

is on the line between $u_{k,0}^{(a)}$ and $u = 0$ in $X_k^{(L)}$.

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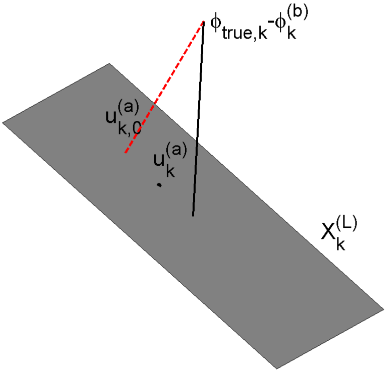

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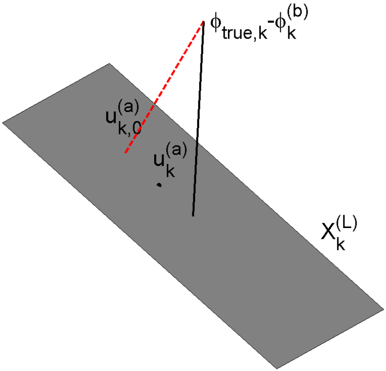

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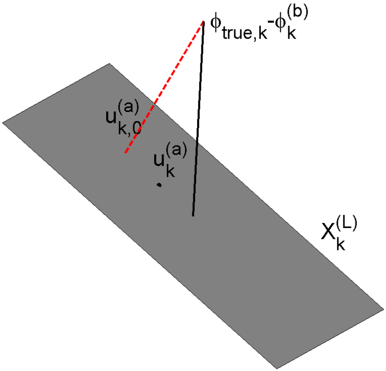

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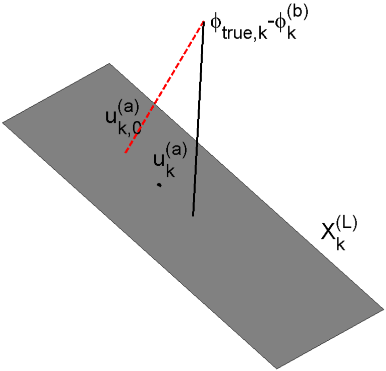

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Error estimates for EnKF

Theorem

Assume that H is injective, that we study true data f_k and consider the EnKF with data term only. Then, the error $E_{k,0}$ in the k-th step of the EnKF is given by

$$E_{k,0} = d_{H^* R^{-1} H}(X_k^{(L)}, \varphi_{true,k} - \varphi^{(b)}).$$

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Assume that H is injective and that we study true data f_k. Then, the error E_k in the k-th step of the EnKF is estimated by

$$\|\varphi_{true,k} - \varphi^{(b)}\|_{H^* R^{-1} H} \geq E_k \geq d_{H^* R^{-1} H}(X_k^{(L)}, \varphi_{true,k} - \varphi^{(b)}).$$

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$$\|\varphi_{true,k} - \varphi^{(b)}\|_{H^* R^{-1} H} \geq E_k \geq d_{H^* R^{-1} H}(X_k^{(L)}, \varphi_{true,k} - \varphi^{(b)}).$$

LEnKF Basic Idea: Localization

- We employ localization:

$$\varphi_k = \varphi_k^{(b)} + B_{loc}H^*\big(R + HB_{loc}H^*\big)^{-1}\big(f_k - H\varphi_k^{(b)}\big)$$

- Here, the localization is given by

$$B_{loc} = C \circ B \tag{18}$$

(where $\circ$ denotes the Schur product, i.e. pointwise matrix multiplication) with

$$C_{j,k} := e^{-|p_i - p_k|^2/\sigma}, \quad j, k = 1, ..., N.$$

- There are different alternative ways how to carry out localization!!

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Outline

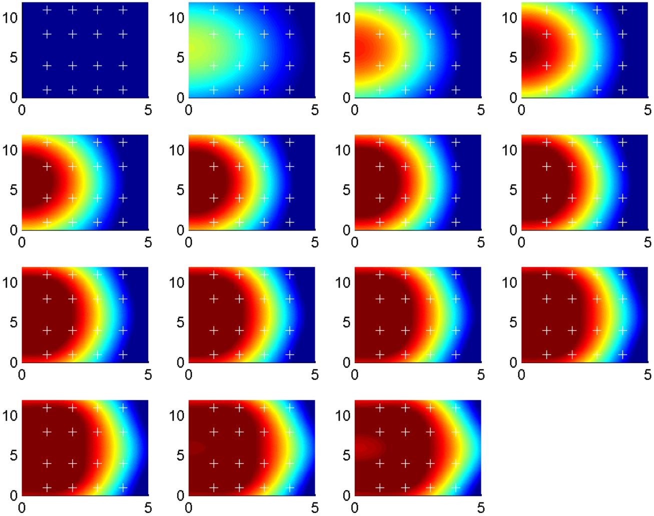
Tikhonov Regularization and 3dVar

Kalman Filter: Update B

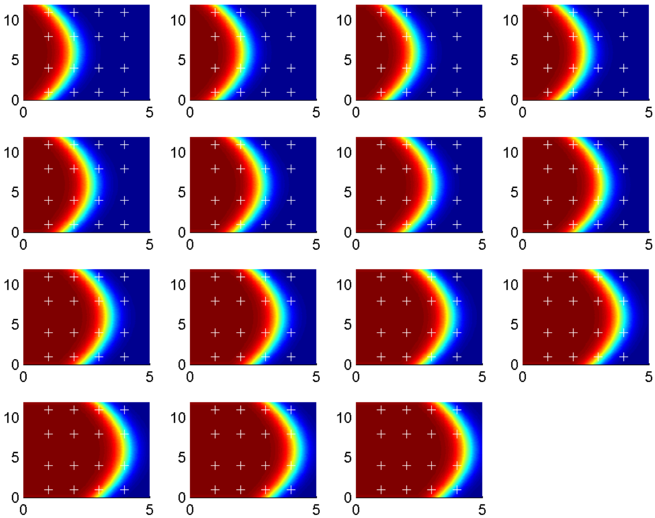
Ensemble Kalman Filter (EnKF) and Local Ensemble Kalman Filter (LEnKF)

Examples for 3dVar, EnKF and LETKF

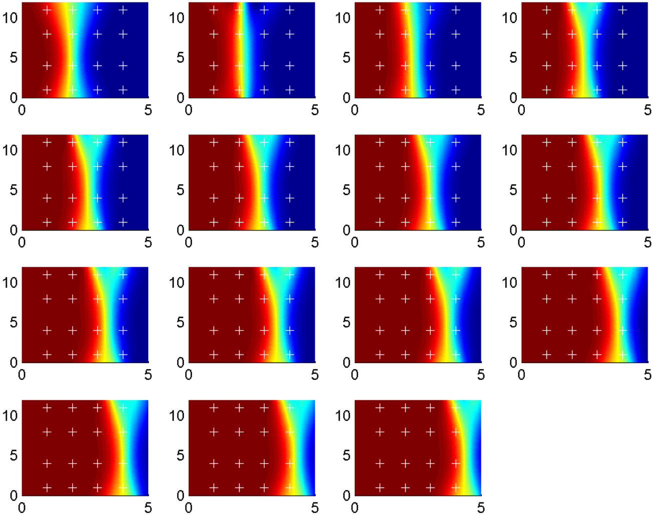
Example 1: 3dVar



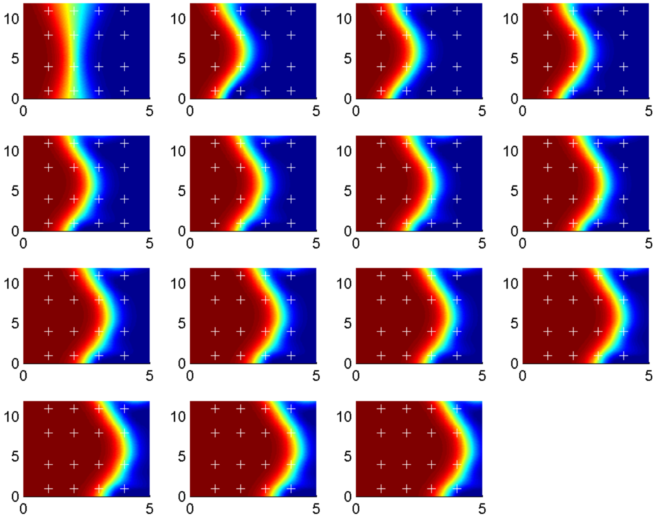
Example 1: Original



Example 1: EnKF



Example 1: LEnKF



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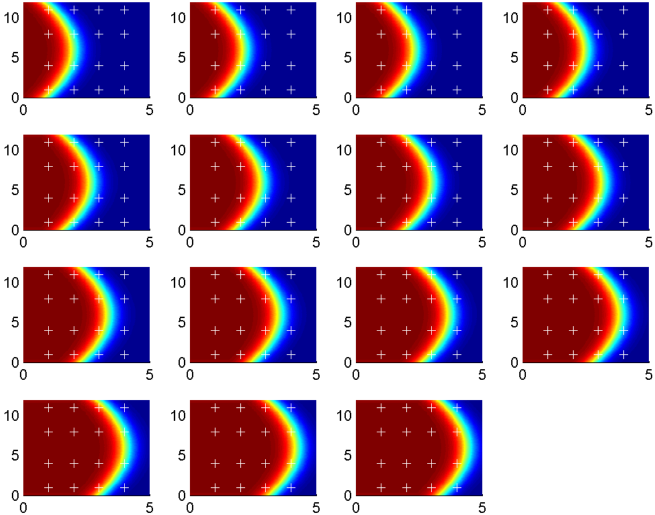
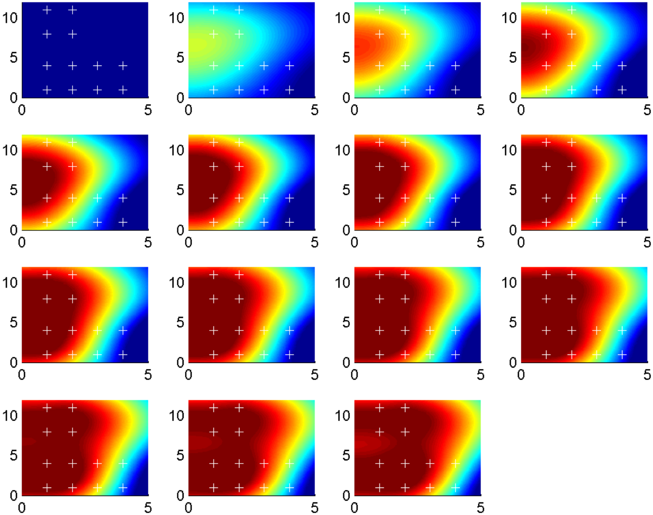


Example 2: 3dVar



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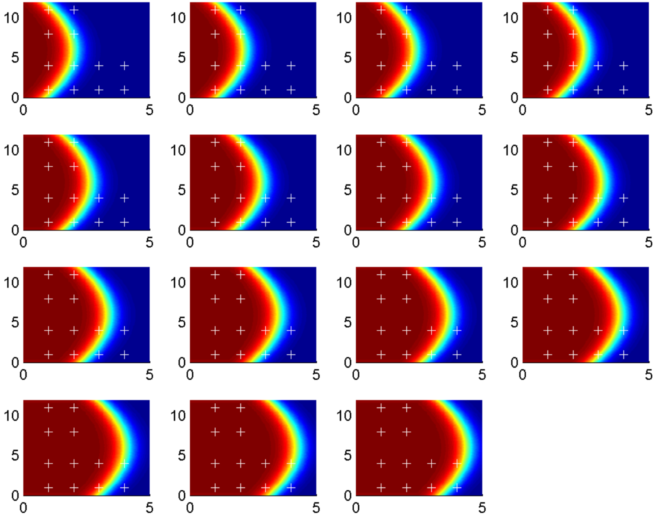

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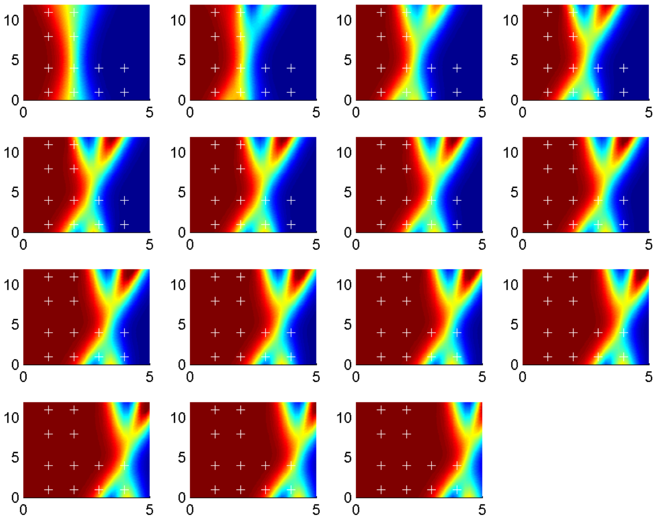

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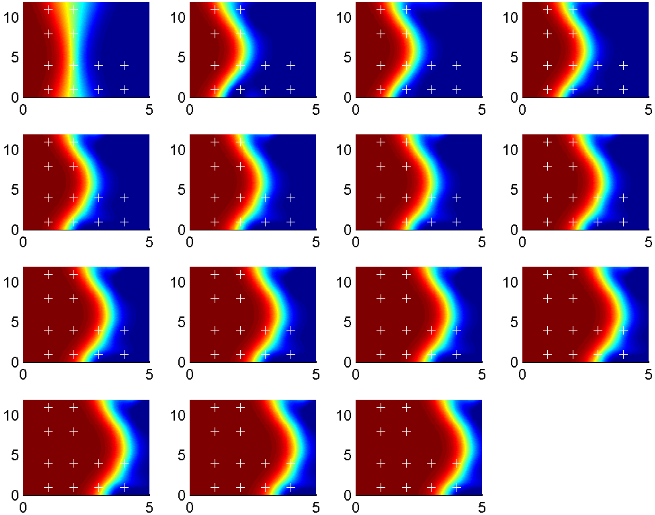

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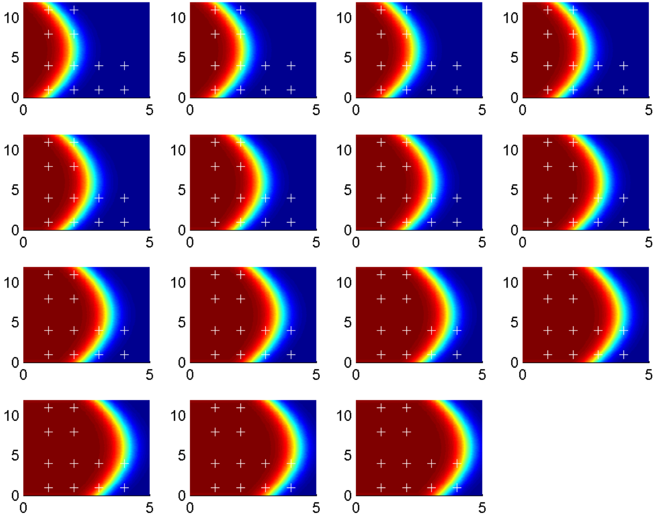
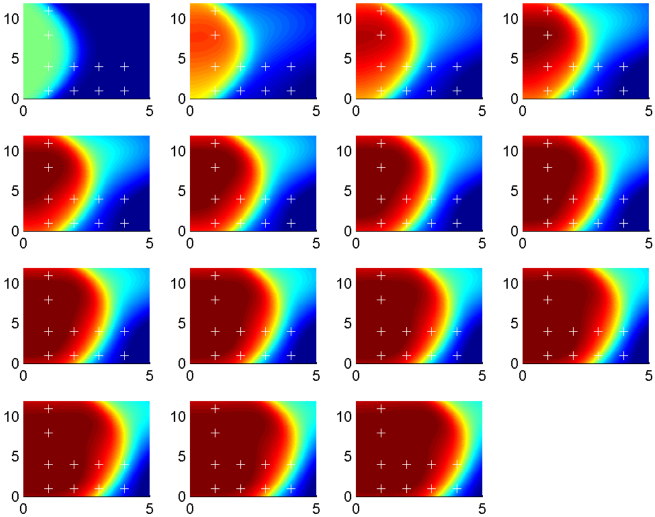
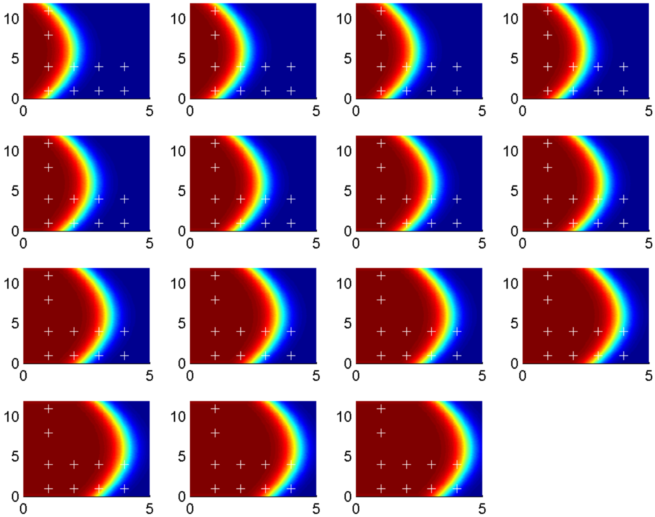


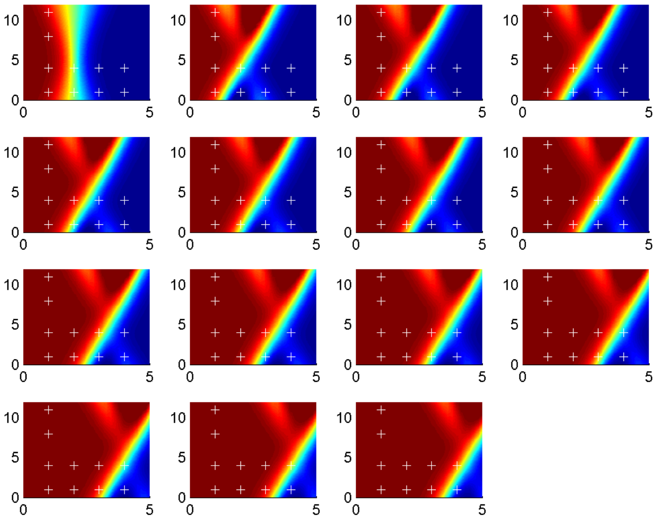
Example 3: 3dVar



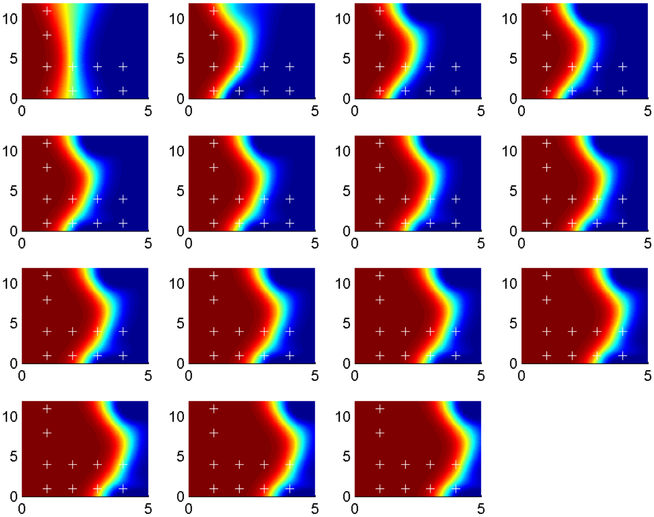
Example 3: Original



Example 3: EnKF



Example 3: LEnKF



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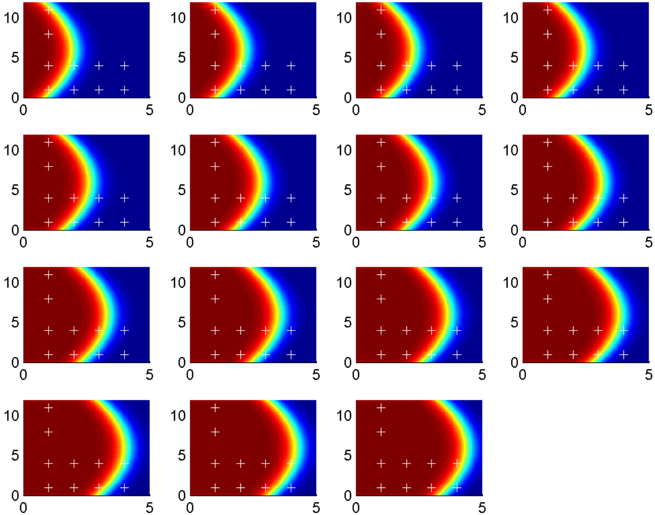

Current work points / scientific and operational questions

1. What type of localization is optimal for our systems?
2. Adaptive localization depending on the data density?
3. Dynamics and update rates, how to choose them?
4. Convection resolving scale and localization strategies?
5. Basic conceptional and convergence questions are unresolved!
6. How to estimate and include model error
7. Localization and nonlocal remote sensing data?

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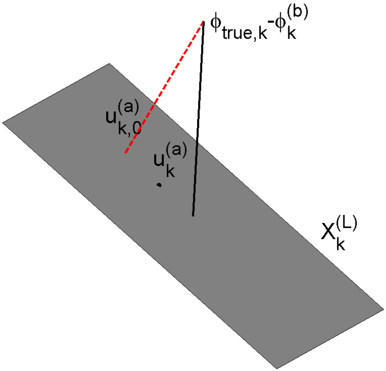
Ensemble Control ...

Control the ensemble

to optimally shape $X_k^{(L)}$ locally ...!



Many Thanks!