

# Estimation de systèmes peu observables en grande dimension par apprentissage statistique

K. KASPER<sup>1</sup>, L. MATHELIN<sup>2</sup> & H. Abou-Kandil<sup>1</sup>

<sup>1</sup>: SATIE - ENS Cachan

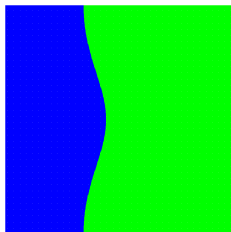
<sup>2</sup>: LIMSI, Orsay

# Motivation: Inverse problems (IP)

Given set of data  $S$  + model  $F$  describing state/solution  $u$  :

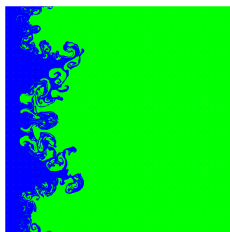
→ estimate parameters  $y$

parameters:  $y \approx Dx$



space sometimes HD  
or temporal fields)

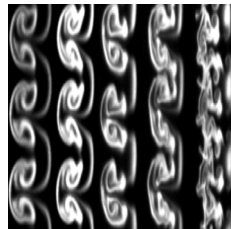
state:  $u \approx Fy$



$F$ : forward model (expensive,  
uncertain, non-linear)

state space is HD

data:  $S \approx Ou$



$O$ : observation operator  
data limited, noisy & indirect

# Motivation

## Goal

Inference of a high-dimensional spatial field from a few sensors.

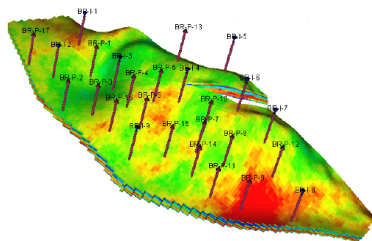


Illustration adapted from Jafarpour & Khaninezhad, 2015.

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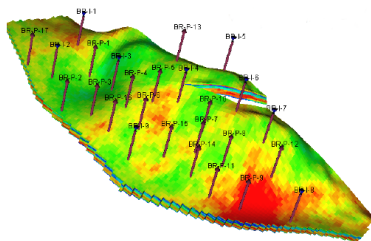


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### Context

- High-dimensional spatial field
- Limited number of sensors
- Limited data

- ➔ Severely ill-posed problem
- ➔ CPU intensive while need for fast solutions

## Standard approach (deterministic framework) — ROM-based state estimation

Derive a reduced-order model:  $\mathbf{y} \approx \hat{\mathbf{y}} = D_{\text{ROM}} \mathbf{x}$ .  $\{D_{\text{ROM}}^{(i)}\}_{i=1}^{n_D}$  typically are PCA modes.  $\mathbf{x}$  is the associated coefficients vector.

From a correlation kernel or a “learning” (unsorted) sequence  $Y := (\mathbf{y}^{(1)} \dots \mathbf{y}^{(n_{\text{snap}})}) \in \mathbb{R}^{n \times n_{\text{snap}}}$ :

$$D_{\text{ROM}} \Sigma V^* \stackrel{\text{thin SVD}}{\approx} Y.$$

For a given number  $n_D$  of retained modes, leads to the best approximation in the following sense:

$$\hat{Y} = D_{\text{ROM}} \hat{X} = \arg \min_{\substack{\tilde{Y} \in \mathbb{R}^{n \times n_{\text{snap}}} \\ \text{rank}[\tilde{Y}] \leq n_D}} \left\| Y - \tilde{Y} \right\|_F \quad \text{with } \hat{X} = \Sigma V^*.$$

- $\mathbf{y} \in \mathbb{R}^n$  field of interest,
- $D_{\text{ROM}} \in \mathbb{R}^{n \times n_D}$  the approximation basis [Dictionary],
- $\mathbf{x} \in \mathbb{R}^{n_D}$  the basis coefficients as estimated from the  $n_s$  sensors,
- $\mathbf{s} \in \mathbb{R}^{n_s}$ , sensor information.

## Standard approach (deterministic framework) — ROM-based state estimation

On site, what is measured is  $\mathbf{s} = O F \mathbf{y} =: G \mathbf{y} \in \mathbb{R}^{n_s}$  only.

$F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ ,  $\mathbf{y} \mapsto \mathbf{u}$ : model operator.

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$G : \mathbb{R}^n \rightarrow \mathbb{R}^{n_s}$ ,  $\mathbf{y} \mapsto \mathbf{s}$ : forward operator.

Observer such that

$$\hat{\mathbf{x}} \in \arg \min_{\tilde{\mathbf{x}} \in \mathbb{R}^{n_D}} \|\mathbf{s} - G D_{\text{ROM}} \tilde{\mathbf{x}}\|_2, \quad [\text{data misfit}]$$

or simply  $\hat{\mathbf{x}} = (G D_{\text{ROM}})^+ \mathbf{s}$ .

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The reconstructed field is finally:

$$\hat{\mathbf{y}} = D_{\text{ROM}} \hat{\mathbf{x}} = D_{\text{ROM}} (G D_{\text{ROM}})^+ \mathbf{s}.$$

$L_{\text{ROM}} := D_{\text{ROM}} (C D_{\text{ROM}})^+$  is the ROM-based lift-up operator.

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$$\hat{\mathbf{x}} \in \arg \min_{\tilde{\mathbf{x}} \in \mathbb{R}^{n_D}} \|\mathbf{s} - G D_{\text{ROM}} \tilde{\mathbf{x}}\|_2, \quad [\text{data misfit}]$$

or simply  $\hat{\mathbf{x}} = (G D_{\text{ROM}})^+ \mathbf{s}$ .  $\leftarrow$  **requires**  $n_s \geq n_D$  (if no additional hyp.)

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# Inversion as statistical inference (SI)

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→ **sparse basis learning** approach

→ Statistical inference restates IP as a **well-posed** extension in a larger space of **probability** distributions

# A dictionary learning algorithm

Without additional hypotheses, impossible to estimate  $n_D > n_s$  modes

→ derive an over-complete dictionary  $D$  for sparse representation of the field  $\mathbf{y} \in \mathcal{M}_y$  to be inferred

$$\mathbf{y} \underset{\epsilon}{\approx} D \mathbf{x}, \quad \mathbf{x} \in \mathbb{R}^{n_D}$$

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→  $n_S$ -sparse approximation

$$\mathbf{y} \underset{\epsilon}{\approx} D \mathbf{x} \quad \text{with} \quad \|\mathbf{x}^{(i)}\|_0 \leq n_S, \quad \forall \mathbf{y} \in \mathcal{M}_y$$

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$$\text{Find } \{D, X\} \in \arg \min_{\tilde{D}, \tilde{X}} \left\| Y - \tilde{D} \tilde{X} \right\|_F \quad \text{s.t.} \quad \|\tilde{\mathbf{x}}^{(i)}\|_0 \leq n_S, \quad \forall i, \quad X := (\mathbf{x}^{(1)} \dots \mathbf{x}^{(n_{\text{snap}})}).$$

# A dictionary learning algorithm

→ use K-SVD algorithm

Repeat

- **Sparse Coding** :  $X \in \arg \min_{\tilde{X}} \|Y - D\tilde{X}\|_F$  s.t.  $\|\tilde{\mathbf{x}}^{(i)}\|_0 \leq n_s, \forall i$ .
- **CodeBook Update** : Update  $D$  and  $X$  in order to lower  $\|Y - DX\|_F$  while maintaining the support of  $\{\mathbf{x}^{(i)}\}_i$ .

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- **CodeBook Update** : Update  $D$  and  $X$  in order to lower  $\|Y - DX\|_F$  while maintaining the support of  $\{\mathbf{x}^{(i)}\}_i$ .

But typically  $\mathbf{x}^{(i)} \in \mathbb{R}^{n_D}$  **cannot** be estimated from measurements: **Observability issue**

→ determine  $D$  given the SI framework for estimating  $\mathbf{x}^{(i)}$  from  $\mathbf{s}^{(i)}$  instead of  $\mathbf{y}^{(i)}$ .  
→ dictionary  $D$  both **accurate** and **observable**:  $D(Y, S)$ .



## → Observability-oriented Dictionary Learning

On-site data:  $\mathbf{s} = G(\mathbf{y})$ .

Let  $\mathcal{M}_{\mathbf{y}} = \{\mathbf{y}_1, \dots, \mathbf{y}_{n_{\text{snap}}}\}$  examples of plausible fields. One looks for a recovery procedure minimizing the *Bayes risk*

$$\begin{aligned}\mathbb{E}_{\mathbf{s}, \mathbf{y}} \left[ \|\mathbf{y} - \hat{\mathbf{y}}(\mathbf{s})\|_2^2 \right] &= \iint \|\mathbf{y} - \hat{\mathbf{y}}(\mathbf{s})\|_2^2 p(\mathbf{s}|\mathbf{y}) p(\mathbf{y}) d\mathbf{s} d\mathbf{y}, \\ &\approx \alpha \left\| Y - \hat{Y}(S) \right\|_F^2. \quad [\text{iid samples}].\end{aligned}$$

with

$$\begin{aligned}\mathbf{y} &\approx \hat{\mathbf{y}} = D\mathbf{x}, \\ \mathbf{s} &\approx \hat{\mathbf{s}} = P(\mathbf{x}) \quad [P: \text{Sparsifying measurement predictor}].\end{aligned}$$

$$\rightarrow \{D, X, P\} \in \arg \min_{\tilde{D}, \tilde{X}, \tilde{P}} \left\| Y - \tilde{D} \tilde{X} (S; \tilde{P}) \right\|_F.$$

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Alternatively:

$$\begin{aligned}\mathbf{y} &\approx \hat{\mathbf{y}} = L(\mathbf{x}) \quad [L: \text{Nonlinear sparsifying lift-up operator}], \\ \mathbf{s} &\approx \hat{\mathbf{s}} = D_{\text{feat}} \mathbf{x}.\end{aligned}$$

$$\rightarrow \{D_{\text{feat}}, X, L\} \in \arg \min_{\tilde{D}_{\text{feat}}, \tilde{X}, \tilde{L}} \left\| Y - \tilde{L}(\tilde{X}(S; \tilde{D}_{\text{feat}})) \right\|_F.$$

## → Observability-oriented Dictionary Learning

$$\begin{aligned} \left\{ \mathbf{x}^{(i)}, D_{\text{feat}} \right\} &\in \arg \min_{\tilde{\mathbf{x}}, \tilde{D}_{\text{feat}}} \left\| \mathbf{s}^{(i)} - \tilde{D}_{\text{feat}} \tilde{\mathbf{x}} \right\|_2^2 & \text{s.t.} & \quad \|\tilde{\mathbf{x}}\|_0 \leq n_s \quad \forall i, \quad \|\tilde{\mathbf{d}}_{\text{feat},l}\|_2 = 1 \quad \forall l, \\ L &\in \arg \min_{\tilde{L}} \left\| Y - \tilde{L}(\tilde{X}) \right\|_F. \end{aligned}$$

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$$\text{Let } \Psi^{(i)} := \left\| \mathbf{s}^{(i)} - \tilde{D}_{\text{feat}} \tilde{\mathbf{x}}^{(i)} \right\|_2^2 + \text{regul}(\tilde{\mathbf{x}}^{(i)})$$

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### → Double-optimization problem

$$\begin{aligned} \{ D_{\text{feat}}, X, L \} &\in \arg \min_{\tilde{D}_{\text{feat}}, \tilde{X}, \tilde{L}} \left\| Y - \tilde{L}(\tilde{X}) \right\|_F, \\ \text{s.t.} \quad \mathbf{c}^{(i)} &:= \frac{\partial \Psi^{(i)}}{\partial \tilde{\mathbf{x}}^{(i)}} = \mathbf{0}, & \forall 1 \leq i \leq n_{\text{snap}}, \\ \frac{\partial \Psi}{\partial \tilde{\mathbf{d}}_{\text{feat}, l}} &= \mathbf{0}, & \text{s.t.} \quad \|\tilde{\mathbf{d}}_{\text{feat}, l}\|_2 = 1, \quad \forall 1 \leq l \leq n_D. \end{aligned}$$

→ consistent and as realistic as possible

## → Observability-oriented Dictionary Learning

$$\left\{ \mathbf{x}^{(i)}, D_{\text{feat}} \right\} \in \arg \min_{\tilde{\mathbf{x}}, \tilde{D}_{\text{feat}}} \left\| \mathbf{s}^{(i)} - \tilde{D}_{\text{feat}} \tilde{\mathbf{x}} \right\|_2^2 \quad \text{s.t.} \quad \left\| \tilde{\mathbf{x}} \right\|_0 \leq n_s \quad \forall i, \quad \left\| \tilde{\mathbf{d}}_{\text{feat}, l} \right\|_2 = 1 \quad \forall l,$$

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$$\text{s.t.} \quad \mathbf{c}^{(i)} := \frac{\partial \Psi^{(i)}}{\partial \tilde{\mathbf{x}}^{(i)}} = \mathbf{0}, \quad \forall 1 \leq i \leq n_{\text{snap}},$$

$$\frac{\partial \Psi}{\partial \tilde{\mathbf{d}}_{\text{feat}, l}} = \mathbf{0}, \quad \text{s.t.} \quad \left\| \tilde{\mathbf{d}}_{\text{feat}, l} \right\|_2 = 1, \quad \forall 1 \leq l \leq n_D.$$

### → consistent and as realistic as possible

- constraints  $\mathbf{c}^{(i)}$  are independent → *parallel solving*,
- e.g., use  $l - \text{BFGS}$ .

## → Observability-oriented Dictionary Learning – Linear framework

On-site data:  $\mathbf{s} = \mathbf{G}\mathbf{y}$ . Linear relationship

$L \equiv D \in \mathbb{R}^{n \times n_D} \in \text{span} \{\mathbf{y}^{(i)}\}$ . Let  $Y \stackrel{\text{QR}}{\equiv} QR$ ,  $D = YB$ .

## → Observability-oriented Dictionary Learning – Linear framework

On-site data:  $\mathbf{s} = G\mathbf{y}$ . **Linear relationship**

$L \equiv D \in \mathbb{R}^{n \times n_D} \in \text{span} \{ \mathbf{y}^{(i)} \}$ . Let  $Y \stackrel{\text{QR}}{\equiv} QR$ ,  $D = YB$ .

Using block-coordinate descent, alternate solve for

- **Observability-oriented Sparse Coding**

$$\mathbf{x}^{(i)} \in \arg \min_{\tilde{\mathbf{x}} \in \mathbb{R}^{n_D}} \left\| \mathbf{s}^{(i)} - D_{\text{feat}} \tilde{\mathbf{x}} \right\|_2, \quad \text{s.t.} \quad \|\mathbf{x}\|_0 \leq n_s,$$

- **Estimation CodeBook Update**

$$D \in \arg \min_{\tilde{D} \in \mathbb{R}^{n \times n_D}} \left\| Y - \tilde{D}X \right\|_F.$$

→ solved directly:  $D \leftarrow YX^+$  [using `qrpinv` (Katsikis *et al.*, 2011)].

→ Recovery error:  $\|R(I_{n_{\text{snap}}} - BX)\|_F$  [inexpensive to evaluate].

- **Feature CodeBook Update**

$$\mathbf{d}_{\text{feat},l} \propto (S - D_{\text{feat},\setminus l} X_{\setminus l}) \hat{\mathbf{x}}_l^T, \quad \|\mathbf{d}_{\text{feat},l}\|_2 = 1, \quad \forall 1 \leq l \leq n_D,$$

with  $\widehat{R\mathbf{b}}_l \hat{\mathbf{x}}_l^{\text{rank-1}} \approx R(I_{n_{\text{snap}}} - B_{\setminus l} X_{\setminus l})$ .

→ consistent and as realistic as possible



# Bayesian Compressive Sensing

Relax  $\|\mathbf{x}\|_0$  (NP-hard optimization problem) in  $\|\cdot\|_1$ .

$$\mathbf{x} \in \arg \min_{\tilde{\mathbf{x}} \in \mathbb{R}^{n_D}} \|\mathbf{s} - D_{\text{feat}} \tilde{\mathbf{x}}\|_2^2 + \tau \|\tilde{\mathbf{x}}\|_1,$$

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Full information on the solution  $\rightarrow$  Bayesian modeling

Independent data during training.

$$\mathbf{x} \in \arg \max_{\tilde{\mathbf{x}} \in \mathbb{R}^{n_D}} q(\tilde{\mathbf{x}}|\mathbf{s}) \propto L(\tilde{\mathbf{x}}|\mathbf{s}) p(\tilde{\mathbf{x}}), \quad \hat{\mathbf{s}} = D_{\text{feat}} \mathbf{x},$$

with

$$L(\mathbf{x}|\mathbf{s}, \beta) \sim \mathcal{N}(\mathbf{s} | D_{\text{feat}} \mathbf{x}, \beta^{-1}),$$

$$p(\mathbf{x}) = \frac{\lambda}{2} \exp\left(-\frac{\lambda}{2} \|\mathbf{x}\|_1\right), \quad [\text{Laplace prior}],$$

$$\tau = \lambda/\beta \quad [\text{sparsity penalty}].$$

## Bayesian Compressive Sensing (cnt'd)

Laplace prior not conjugate to the likelihood model  
Sparsity regularization penalty  $\tau$  unknown }  $\rightarrow$  hierarchical formulation

$$p(\mathbf{x}|\boldsymbol{\gamma}) = \prod_{i=1}^{n_D} \mathcal{N}(x_i|0, \gamma_i), \quad \boldsymbol{\gamma} = (\gamma_1 \dots \gamma_{n_D}), \quad (1)$$

$$p(\gamma_i|\lambda) = \frac{\lambda}{2} \exp\left(-\frac{\lambda \gamma_i}{2}\right), \quad (2)$$

$$p(\lambda|\nu) = \Gamma(\lambda|\nu/2, \nu/2).$$

Each of the  $n_D$  independent hyperparameters  $\gamma_i$  controls the strength of the prior  $\rightarrow$  introduces sparsity in the model.

# Sequential Sparse Bayesian Learning

→ three-stage hierarchy. Eqs. (1)-(2) result in a Laplace distribution  $p(\mathbf{x}|\lambda)$ ,

→  $q(\mathbf{x}|\mathbf{s}, \gamma, \beta, \lambda)$  is a multivariate Gaussian distribution  $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ ,

$$\boldsymbol{\mu} = \beta \boldsymbol{\Sigma} D_{\text{feat}}^T \mathbf{s}, \quad \boldsymbol{\Sigma} = \left( \beta D_{\text{feat}}^T D_{\text{feat}} + \boldsymbol{\Lambda} \right)^{-1}, \quad \boldsymbol{\Lambda} = \text{diag} \left( \gamma_1^{-1}, \dots, \gamma_{n_D}^{-1} \right).$$

Follows Babacan *et al.* (2010).

Hyperparameters maximize the (log-) marginal likelihood

$$\log p(\mathbf{s}, \gamma, \beta, \lambda) = \log \int p(\mathbf{s}|\mathbf{x}, \beta) p(\mathbf{x}|\gamma) p(\gamma|\lambda) p(\lambda) p(\beta) d\mathbf{x}$$

→ MAP estimate:  $\hat{\mathbf{y}} = D \boldsymbol{\mu}$ .

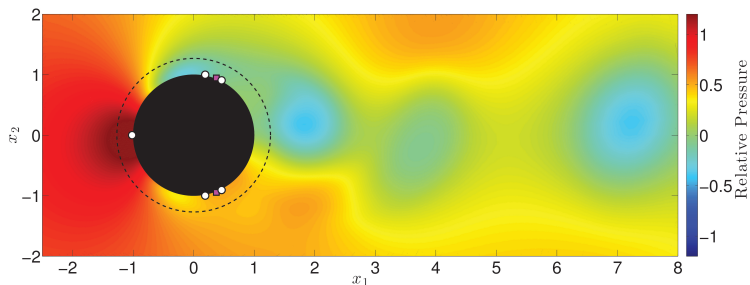
## 1 Basis learning **[offline]**

- ▶ Form a snapshot matrix  $Y$  of expected realizations of the field and corresponding matrix  $S$ ,
- ▶ Given the sensors, learn representation dictionaries  $D$  (and  $D_{\text{feat}}$ ) using Sparse Bayesian Dictionary Learning,

## 2 Field reconstruction **[online]**

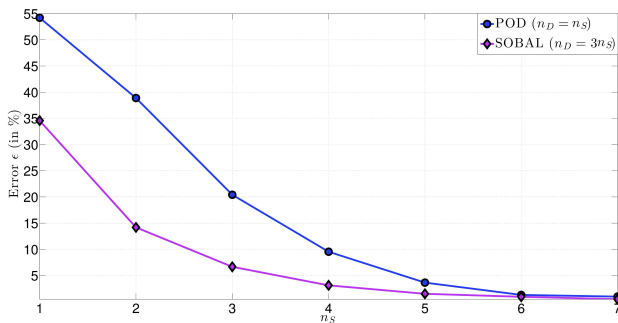
- ▶ Use SBL with the measure  $\mathbf{s}$  to estimate  $\mathbf{x} \sim \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma)$ .
- ▶ Reconstruct the MAP total field from  $\hat{\mathbf{y}} = D\boldsymbol{\mu}$  or use Markov chain Monte Carlo.

## Numerical experiment: pressure field



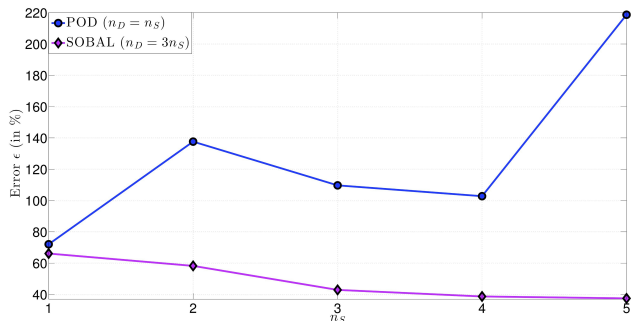
- $\mathbf{y}$ : pressure field
- $\mathbf{s}$ : measurements at the surface ( $n_s \leq 5$ )

## Observability issue. Full information: $\mathbf{s} \equiv \mathbf{y}$



→ significantly better  $L^2$ -reconstruction performance than PCA/KL.

## Observability issue. Sensor information only

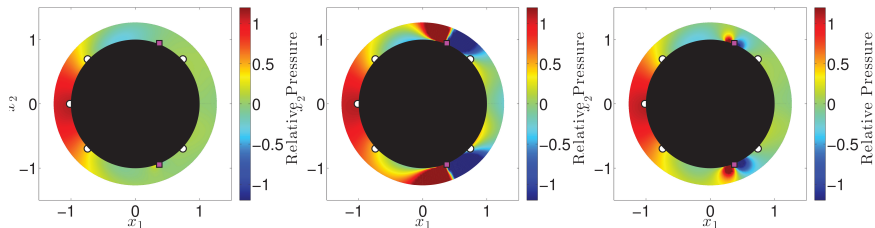


→ significantly better  $L^2$ -reconstruction performance than PCA/KL.

→ PCA coefficients are not accurately estimated from the sensors.



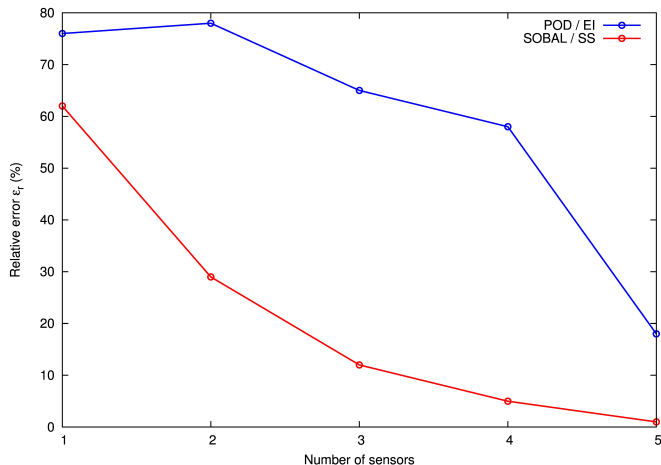
# Reconstruction



Relative pressure field. Exact (left), estimated from PCA/KL (middle), estimated from present approach (right).

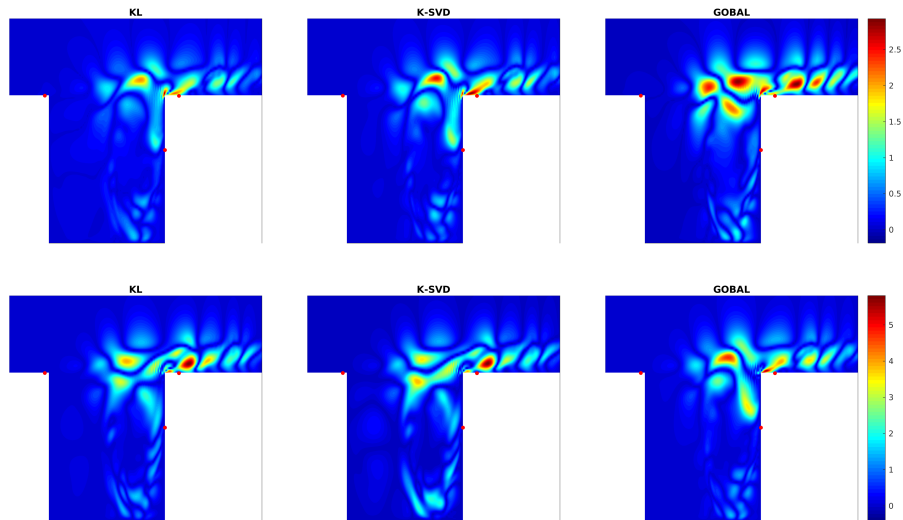
→ Much better reconstruction performance.

## Combined with SensorSpace...

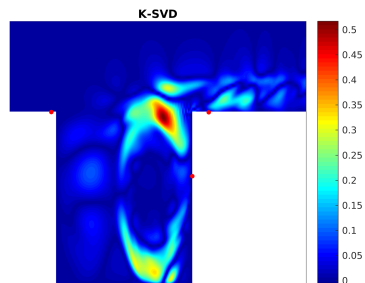
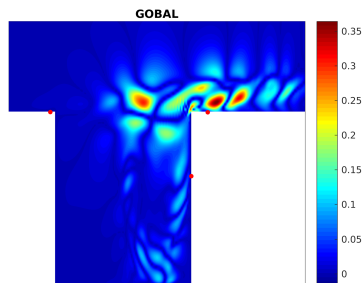
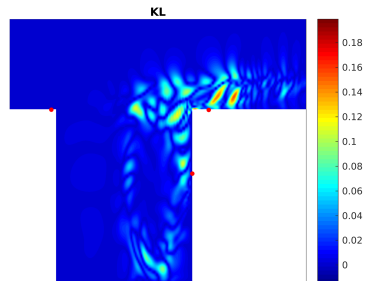
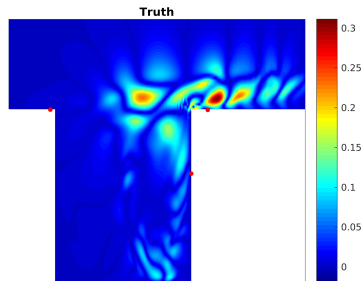


→ PCA/Effective Independence compared to SOBAL / SensorSpace.

# Cavity flow – Dictionary



# Recovery performance – 3 sensors



## Closing remarks

- Offline/Online strategy for inference. First learn about the system at hand, then exploit,
- Basis learning philosophy is a key for a *realistic* and successful approach,
- Need to balance between representation accuracy and observability when using a dictionary  
→ *observability-oriented sparse Bayesian learning*.

## Closing remarks

- Offline/Online strategy for inference. First learn about the system at hand, then exploit,
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→ *observability-oriented sparse Bayesian learning*.

### On-going efforts:

- High-dimensional fields, nonlinear observation operator,
- Combined with an assimilation technique, e.g., sparsity exploiting EnKF.