The Reduced Basis Ensemble Kalman Method :

an Iterative Regularization Method

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OUTLINE

ASYNCHRONOUS DATA ASSIMILATION : AN INVERSE PROBLEM

$$\boxed{y = \mathbf{L}\, u_{\text{TRUE}} + \epsilon}$$

ASYNCHRONOUS MEASUREMENTS

ASYNCHRONOUS DATA ASSIMILATION : AN INVERSE PROBLEM

$$\boxed{\boldsymbol{y} = \mathbf{L}\, u_{\mathrm{TRUE}} + \boldsymbol{\epsilon}}$$

ASYNCHRONOUS MEASUREMENTS

$$\boxed{(\mathcal{M}_{\boldsymbol{\mu}} u, \psi) = 0 \quad \forall \psi \in \mathcal{Y}}$$

PHYSICAL MODEL

ASYNCHRONOUS DATA ASSIMILATION : AN INVERSE PROBLEM

$\boxed{\boldsymbol{y} = \mathbf{L}\,u_{\mathrm{TRUE}} + \boldsymbol{\epsilon}}$

ASYNCHRONOUS MEASUREMENTS

DATA ASSIMILATION

$\boxed{(\mathcal{M}_{\boldsymbol{\mu}} u, \psi) = 0 \quad \forall \psi \in \mathcal{Y}}$

PHYSICAL MODEL

$\boxed{u_{\mathrm{OPT}}, \boldsymbol{\mu}_{\mathrm{OPT}}}$

STATE/PARAMETER ESTIMATION

[SEB10]

OUTLINE

VARIATIONAL DATA ASSIMILATION : CONSTRAINED MINIMIZATION

$$\min_{\boldsymbol{\mu}\in\mathcal{P}} \mathcal{J}(\boldsymbol{\mu}\,|\boldsymbol{y}) \coloneqq \frac{1}{2}\boxed{\|\boldsymbol{y}-\mathbf{L}\,u\|^2_{\Sigma^{-1}}}$$

DATA MISFIT

such that $\boxed{\left(\mathcal{M}_{\boldsymbol{\mu}}u,\psi\right)=0 \quad \forall\psi\in\mathcal{Y}}$

WEAK MODEL

where:

$\boldsymbol{y} \;= \mathbf{L}\,u_{\mathrm{TRUE}}+\boldsymbol{\epsilon}$ *with noise* $\boldsymbol{\epsilon}\sim\mathcal{N}(0,\Sigma)$

VARIATIONAL DATA ASSIMILATION : REGULARIZED

$$\min_{\boldsymbol{\mu}\in\mathcal{P}} \mathcal{J}(\boldsymbol{\mu}\,|\boldsymbol{y}) := \frac{1}{2}\underbrace{\boxed{\|\boldsymbol{y}-\mathbf{L}u\|^2_{\Sigma^{-1}}}}_{\text{DATA MISFIT}} + \underbrace{\boxed{\mathcal{T}(\boldsymbol{\mu})}}_{\text{STABILIZATION}} \quad \text{such that} \quad \underbrace{\boxed{(\mathcal{M}_{\boldsymbol{\mu}}u,\psi)=0 \quad \forall\psi\in\mathcal{Y}}}_{\text{WEAK MODEL}}$$

where:

$$\boldsymbol{y} = \mathbf{L}\,u_{\text{TRUE}} + \boldsymbol{\epsilon} \quad \textit{with noise} \quad \boldsymbol{\epsilon}\sim\mathcal{N}(0,\Sigma)$$

[TC91]

VARIATIONAL DATA ASSIMILATION : UNREGULARIZED

$$\min_{\boldsymbol{\mu}\in\mathcal{P}} \mathcal{J}(\boldsymbol{\mu}\,|\boldsymbol{y}) := \frac{1}{2}\boxed{\|\boldsymbol{y}-\mathbf{L}\,u\|^2_{\Sigma^{-1}}}$$

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such that $\boxed{(\mathcal{M}_{\boldsymbol{\mu}}u,\psi)=0 \quad \forall\psi\in\mathcal{Y}}$

WEAK MODEL

where:

$$\boldsymbol{y} = \mathbf{L}\,u_{\mathrm{TRUE}} + \boldsymbol{\epsilon} \quad \textit{with noise} \quad \boldsymbol{\epsilon}\sim\mathcal{N}(0,\Sigma)$$

the solution of the un-regularized problem can be obtained employing an iterative regularization methods

[KNS08]

$$\boldsymbol{\mu}_{\mathrm{k}+1} = \boldsymbol{\mu}_{\mathrm{k}} + \mathcal{G}_{\mathrm{k}}(\boldsymbol{\mu}_{\mathrm{k}},\boldsymbol{y}) \longleftarrow$$ Landweber iterations

[Lan51]

VARIATIONAL DATA ASSIMILATION : UNREGULARIZED

$$\min_{\boldsymbol{\mu}\in\mathcal{P}} \mathcal{J}(\boldsymbol{\mu}\,|\boldsymbol{y}) := \frac{1}{2}\boxed{\|\boldsymbol{y}-\mathbf{L}\,u\|^2_{\Sigma^{-1}}}$$

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WEAK MODEL

where:

$\boldsymbol{y} = \mathbf{L}\,u_{\text{TRUE}} + \boldsymbol{\epsilon}$ *with noise* $\boldsymbol{\epsilon}\sim\mathcal{N}(0,\Sigma)$

the solution of the un-regularized problem can be obtained employing an iterative regularization methods; those can be implemented via

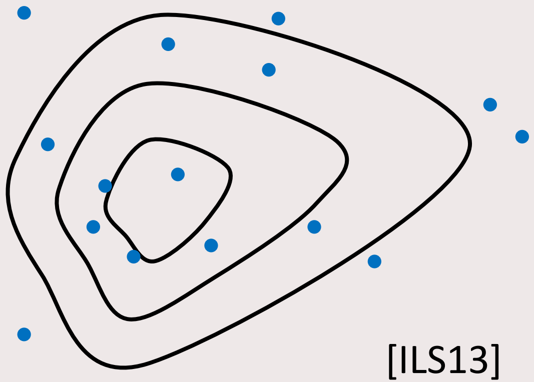
→ Local approaches (Newton's type methods)

→ Global approaches (Particles based methods)

THE ENSEMBLE KALMAN METHOD

We sample a particle ensemble of size J from a prior distribution π_0 and update their positions as follows:

- $\boldsymbol{\mu}_0^{(j)} \sim \pi_0 := e^{-\mathcal{T}(\boldsymbol{\mu})}$



[ILS13]

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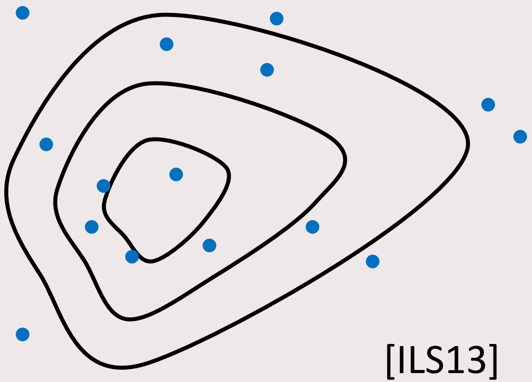
For $n = 0,1, \ldots$

i) Compute the model solution for each particle $\boldsymbol{\mu}_n^{(j)}$:

$$u_n^{(j)} \in \mathcal{X} \quad \text{such that} \quad \left(\mathcal{M}_{\boldsymbol{\mu}_n^{(j)}} u_n^{(j)}, \psi\right) = 0 \quad \forall \psi \in \mathcal{Y}$$



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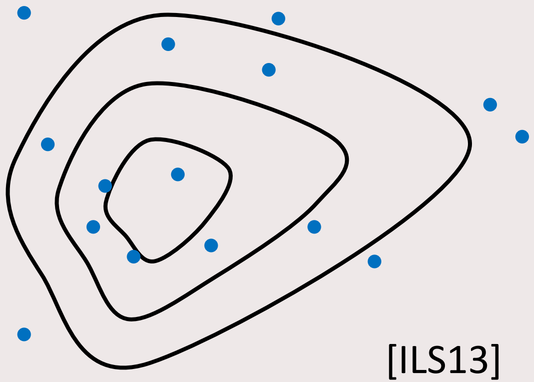
ii) Compute the correlation matrices :

$$P_n := \mathrm{sum}\left(\mathbf{L}\,u_n^{(j)} \otimes \mathbf{L}\,u_n^{(j)} - \mathbf{L}\bar{u}_n \otimes \mathbf{L}\bar{u}_n\right) \cdot (J-1)^{-1}$$

$$Q_n := \mathrm{sum}\left(\boldsymbol{\mu}_n^{(j)} \otimes \mathbf{L}\,u_n^{(j)} - \bar{\boldsymbol{\mu}}_n \otimes \mathbf{L}\bar{u}_n\right) \cdot (J-1)^{-1}$$



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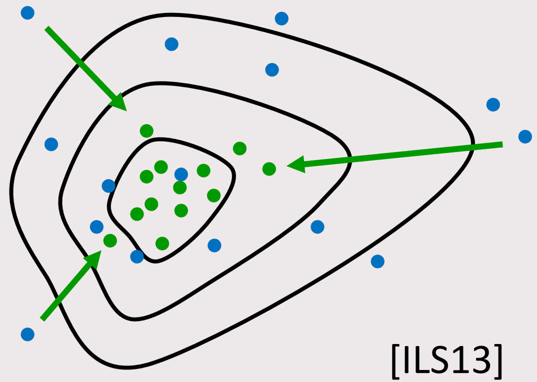
$$\boldsymbol{\mu}_{n+1}^{(j)} = \boldsymbol{\mu}_n^{(j)} + Q_n(\Sigma + P_n)^{-1}\left(\boldsymbol{y} - \mathbf{L}\,u_n^{(j)}\right)$$

- $\boldsymbol{\mu}_0^{(j)} \sim \pi_0 := e^{-\mathcal{T}(\boldsymbol{\mu})}$
- $\boldsymbol{\mu}_{n+1}^{(j)} \sim \pi_0 \cdot \left(e^{-\mathcal{J}(\boldsymbol{\mu}|\boldsymbol{y})}\right)^{n+1}$



[ILS13]

OUTLINE

PARABOLIC pPDEs : SPACE-TIME CONSTRAINT

$\partial_t u(\boldsymbol{x}, t; \boldsymbol{\mu}) + \mathcal{F}_{\boldsymbol{\mu}} u(\boldsymbol{x}, t; \boldsymbol{\mu}) = 0$ for any $\boldsymbol{x} \in \Omega \subset \mathbb{R}^d$ and $t \in I \coloneqq [0, T]$

$u(\boldsymbol{x}, 0; \boldsymbol{\mu}) - u_0(\boldsymbol{x}, \boldsymbol{\mu}) = 0$ for any $\boldsymbol{x} \in \Omega \subset \mathbb{R}^d$

PARABOLIC pPDEs : SPACE-TIME CONSTRAINT

$$\partial_t u(\boldsymbol{x},t;\boldsymbol{\mu}) + \mathcal{F}_{\boldsymbol{\mu}} u(\boldsymbol{x},t;\boldsymbol{\mu}) = 0 \qquad \text{for any } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d \text{ and } t \in I \coloneqq [0,T]$$

$$u(\boldsymbol{x},0;\boldsymbol{\mu}) - u_0(\boldsymbol{x},\boldsymbol{\mu}) = 0 \qquad \text{for any } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d$$

to which corresponds the variational formulation:

$$\int_I \left\langle \partial_t u(\boldsymbol{x},t;\boldsymbol{\mu}) + \mathcal{F}_{\boldsymbol{\mu}} u(\boldsymbol{x},t;\boldsymbol{\mu}), v(\boldsymbol{x},t) \right\rangle_{\mathcal{H}} dt = 0 \qquad \forall \; v(\boldsymbol{x},t) \in L^2(I,\mathcal{V})$$

$$\langle u(\boldsymbol{x},0;\boldsymbol{\mu}) - u_0(\boldsymbol{x},\boldsymbol{\mu}), \xi(\boldsymbol{x}) \rangle_{\mathcal{H}} = 0 \qquad \forall \; \xi(\boldsymbol{x}) \in \mathcal{H}$$

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$$\begin{array}{lllll} \displaystyle\int_I \left\langle \partial_t u(\boldsymbol{x},t;\boldsymbol{\mu}) + \mathcal{F}_{\boldsymbol{\mu}} u(\boldsymbol{x},t;\boldsymbol{\mu}), v(\boldsymbol{x},t) \right\rangle_{\mathcal{H}} dt = 0 & \forall & v(\boldsymbol{x},t) & \in & L^2(I,\mathcal{V}) \\ \langle u(\boldsymbol{x},0;\boldsymbol{\mu}) - u_0(\boldsymbol{x},\boldsymbol{\mu}), \xi(\boldsymbol{x}) \rangle_{\mathcal{H}} = 0 & \forall & \xi(\boldsymbol{x}) & \in & \mathcal{H} \\ & & \psi & & \mathcal{Y} \end{array}$$

PARABOLIC pPDEs : SPACE-TIME CONSTRAINT

$\partial_t u(\boldsymbol{x},t;\boldsymbol{\mu}) + \mathcal{F}_{\boldsymbol{\mu}} u(\boldsymbol{x},t;\boldsymbol{\mu}) = 0$ for any $\boldsymbol{x} \in \Omega \subset \mathbb{R}^d$ and $t \in I \coloneqq [0,T]$

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$$\langle u(\boldsymbol{x},0;\boldsymbol{\mu}) - u_0(\boldsymbol{x},\boldsymbol{\mu}), \xi(\boldsymbol{x}) \rangle_{\mathcal{H}} = 0 \qquad \forall\ \xi(\boldsymbol{x}) \in \mathcal{H}$$

$$\underbrace{\boxed{v(\boldsymbol{x},t),\ \xi(\boldsymbol{x})}}_{\psi} \in \underbrace{\boxed{L^2(I,\mathcal{V}),\ \mathcal{H}}}_{\mathcal{Y}}$$

that can be written as:

$$\boxed{\left(\mathcal{M}_{\boldsymbol{\mu}} u, \psi\right)_{\mathcal{Y}} = 0 \quad \forall \psi \in \mathcal{Y}}$$

SPACE-TIME WEAK MODEL

[UP14]

NUMERICAL APPROXIMATION

the infinite dimensional problem can be approximated by Petrov-Galerkin projection

$$\text{find } u_\varepsilon \in \mathcal{X}_\varepsilon \subset \mathcal{X} \quad \text{such that} \quad (\mathcal{M}_{\boldsymbol{\mu}} u_\varepsilon, \psi_i) = 0 \quad \text{for all } \psi_i \in \mathcal{Y}_\varepsilon \subset \mathcal{Y}$$

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where

$\mathcal{X}_\varepsilon$: **trial space** $\longleftarrow$ must ensure good approximation

$\mathcal{Y}_\varepsilon$: **test space** $\longleftarrow$ must ensure proper stability

NUMERICAL APPROXIMATION : REDUCED BASIS METHODS

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where

$\mathcal{X}_\varepsilon$: **trial space** ⟵ must ensure good approximation

$\mathcal{Y}_\varepsilon$: **test space** ⟵ must ensure proper stability

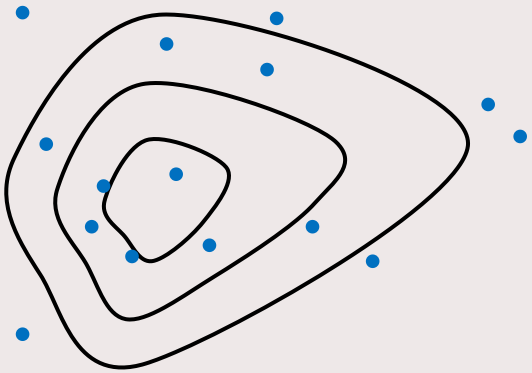
Reduced Basis (**RB**) methods employ a set of pre-computed solutions to choose an optimal couple $(\mathcal{X}_\varepsilon, \mathcal{Y}_\varepsilon)$. [BHL93] [HO08]

OUTLINE

1. INTRODUCTION
2. VARIATIONAL METHODS
3. MODEL APPROXIMATION
4. **THE REDUCED BASIS ENSEMBLE KALMAN METHOD**
5. NUMERICAL EXPERIMENTS
6. CONCLUSIONS

THE (REDUCED BASIS) ENSEMBLE KALMAN METHOD

We sample a particle ensemble of size J from a prior distribution π_0 and update their positions as follows:



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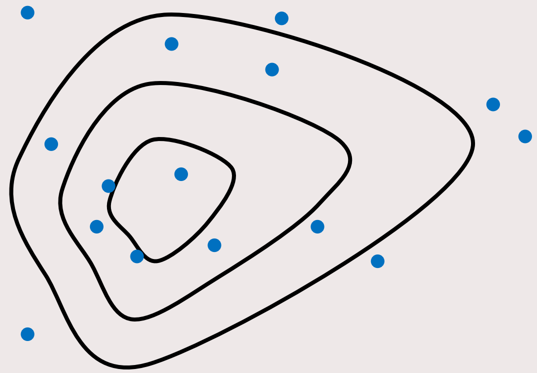


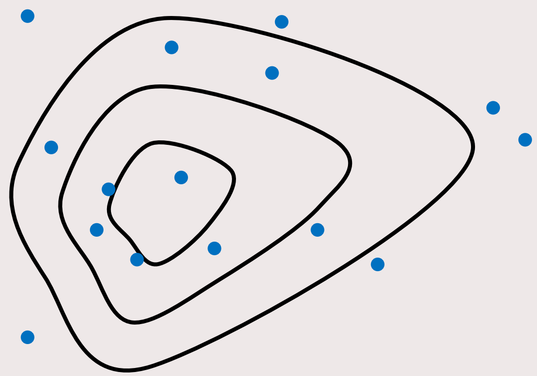
THE REDUCED BASIS ENSEMBLE KALMAN METHOD

We sample a particle ensemble of size J from a prior distribution π_0 and update their positions as follows:

For $n = 0,1,\dots$

i) Compute the model solution for each particle $\boldsymbol{\mu}_n^{(j)}$:

$$u_{\varepsilon,n}^{(j)} \in \mathcal{X}_\varepsilon \quad \text{such that} \quad \left(\mathcal{M}_{\boldsymbol{\mu}_n^{(j)}} u_{\varepsilon,n}^{(j)}, \psi_i\right) = 0 \quad \forall \psi_i \in \mathcal{Y}_\varepsilon$$



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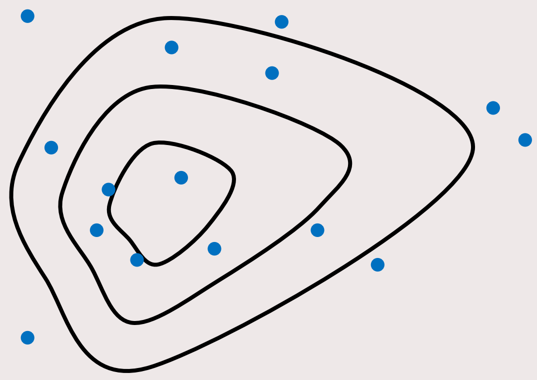

THE REDUCED BASIS ENSEMBLE KALMAN METHOD

We sample a particle ensemble of size J from a prior distribution π_0 and update their positions as follows:

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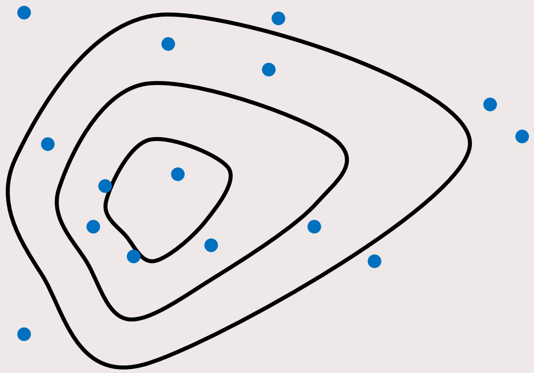
$$P_{\varepsilon,n} \coloneqq \mathrm{sum}\left(\mathbf{L}\,u_{\varepsilon,n}^{(j)} \otimes \mathbf{L}\,u_{\varepsilon,n}^{(j)} - \mathbf{L}\bar{u}_{\varepsilon,n} \otimes \mathbf{L}\bar{u}_{\varepsilon,n}\right) \cdot (J-1)^{-1}$$

$$Q_{\varepsilon,n} \coloneqq \mathrm{sum}\left(\boldsymbol{\mu}_n^{(j)} \otimes \mathbf{L}\,u_{\varepsilon,n}^{(j)} - \bar{\boldsymbol{\mu}}_n \otimes \mathbf{L}\bar{u}_{\varepsilon,n}\right) \cdot (J-1)^{-1}$$



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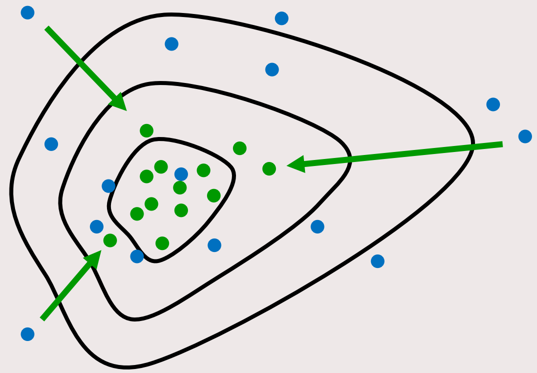

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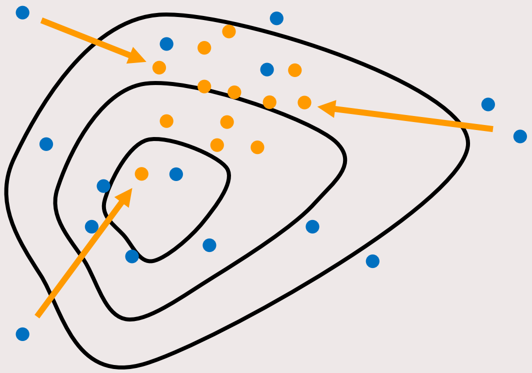

THE REDUCED BASIS ENSEMBLE KALMAN METHOD

We sample a particle ensemble of size J from a prior distribution π_0 and update their positions as follows:

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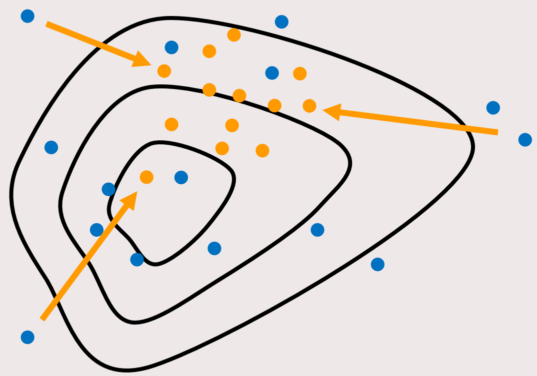
iii) Update each particle $\boldsymbol{\mu}_n^{(j)}$ in the ensemble:

$$\boldsymbol{\mu}_{n+1}^{(j)} \overset{!}{\neq} \boldsymbol{\mu}_n^{(j)} + Q_{\varepsilon,n}(\Sigma + P_{\varepsilon,n})^{-1}\left(\boldsymbol{y} - \mathbf{L}\, u_{\varepsilon,n}^{(j)}\right)$$

Such an iteration would not converge to $\boldsymbol{\mu}_{\mathrm{OPT}}$ because

$$\min_{\boldsymbol{\mu}\in\mathcal{P}} \frac{1}{2}\|\boldsymbol{y} - \mathbf{L}\, u\|_{\Sigma^{-1}}^2 \neq \min_{\boldsymbol{\mu}\in\mathcal{P}} \frac{1}{2}\|\boldsymbol{y} - \mathbf{L}\, u_\varepsilon\|_{\Sigma^{-1}}^2$$



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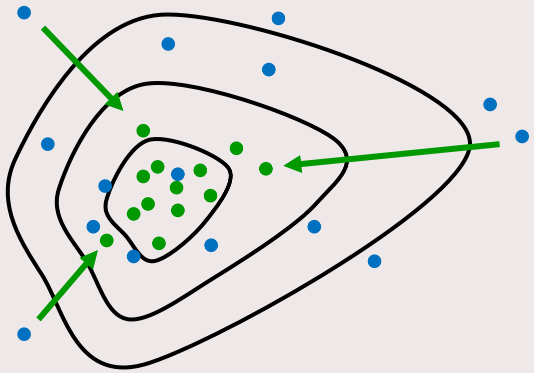
where

$$\boldsymbol{\delta}_{\varepsilon,n} \coloneqq \frac{1}{J} \cdot \mathrm{sum}\left(\mathbf{L}\,(u_{\varepsilon,n}^{(j)} - u_n^{(j)})\right)$$

$$\Gamma_{\varepsilon,n} \coloneqq \frac{1}{J-1} \cdot \mathrm{sum}\left(\mathbf{L}\,(u_{\varepsilon,n}^{(j)} - u_n^{(j)}) \otimes \mathbf{L}\,(u_{\varepsilon,n}^{(j)} - u_n^{(j)}) - \boldsymbol{\delta}_{\varepsilon,n} \otimes \boldsymbol{\delta}_{\varepsilon,n}\right)$$



[PMQ16]
[Cal+18]

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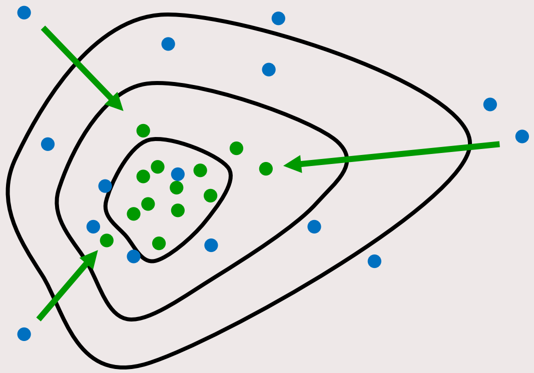
$$\Gamma_{\varepsilon,0} := \frac{1}{J-1} \cdot \mathrm{sum}\left(\mathbf{L}\,(u_{\varepsilon,0}^{(j)} - u_0^{(j)}) \otimes \mathbf{L}\,(u_{\varepsilon,0}^{(j)} - u_0^{(j)}) - \boldsymbol{\delta}_{\varepsilon,0} \otimes \boldsymbol{\delta}_{\varepsilon,0}\right)$$

$\longleftarrow$ same $u_0^{(j)}$ used for training the RB model



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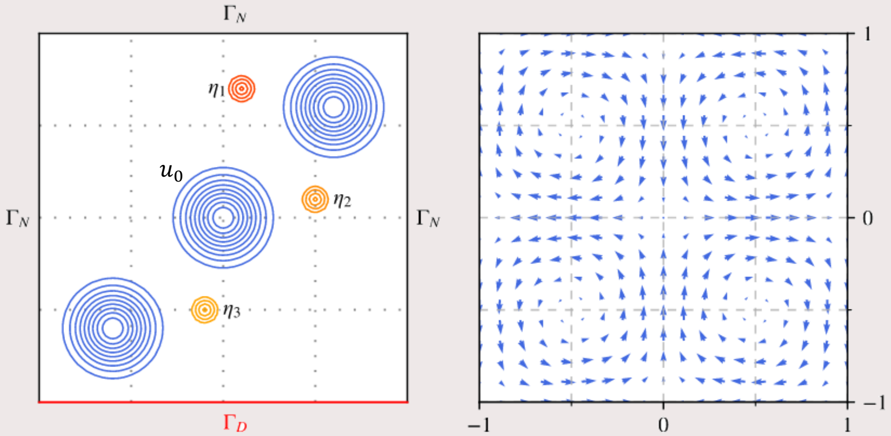
ADVECTION-DISPERSION PROBLEM

unknown

$$\frac{\partial u}{\partial t} - \boldsymbol{\mu} \cdot \Delta u(t) + \boldsymbol{v} \cdot \nabla u(t) = 0 \quad \text{on } \Omega \coloneqq (-1,+1)^2 \qquad \text{with} \qquad \boldsymbol{v} = \begin{bmatrix} +\sin(\pi x_1)\cos(\pi x_2) \\ -\cos(\pi x_1)\sin(\pi x_2) \end{bmatrix}$$

$$u(0) = u_0$$



[Kär+18]

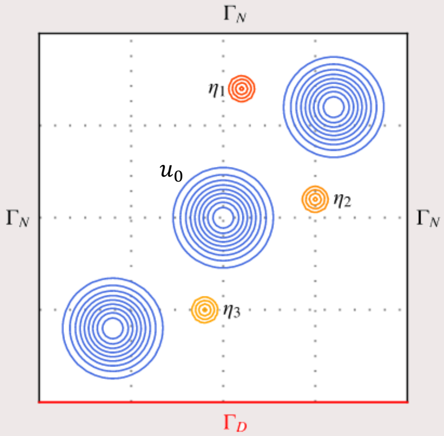
ADVECTION-DISPERSION PROBLEM

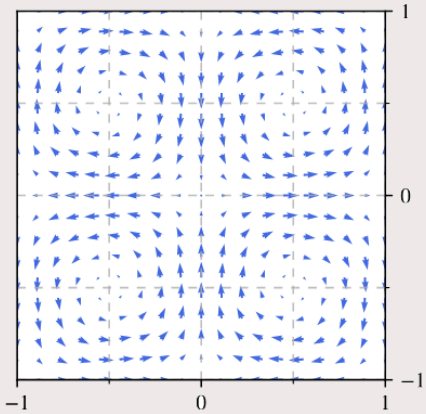
$$\frac{\partial u}{\partial t} - \boldsymbol{\mu} \cdot \Delta u(t) + \boldsymbol{v} \cdot \boldsymbol{\nabla} u(t) = 0 \quad \text{on } \Omega \coloneqq (-1,+1)^2 \quad \text{with} \quad \boldsymbol{v} = \begin{bmatrix} +\sin(\pi x_1)\cos(\pi x_2) \\ -\cos(\pi x_1)\sin(\pi x_2) \end{bmatrix}$$

$$u(0) = u_0$$

we consider:

- 3 sensor locations
- 40 time-activations per sensor
- $t \in (0, 2.4)$
- $\boldsymbol{\mu} \in [1/50, 1/10]$



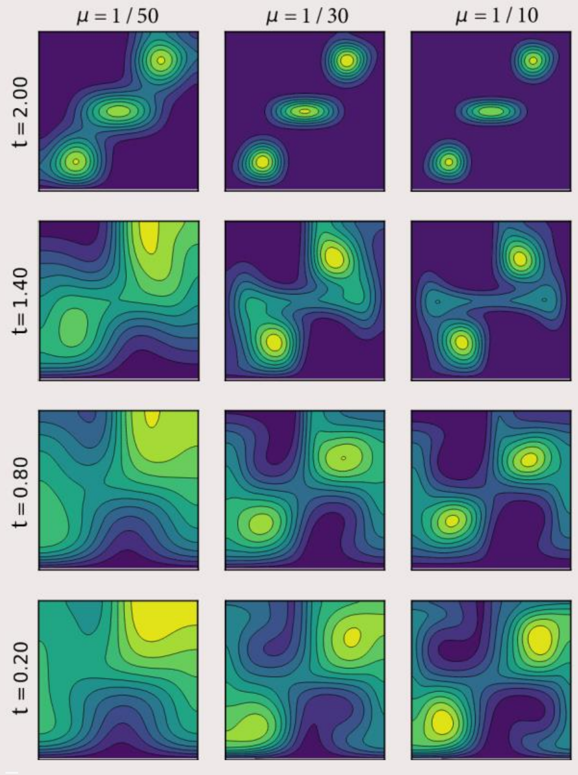


MODEL ORDER REDUCTION

considering a fine **FE discretization** as exact model

FE dofs spatial discretization = 10100 (P2-P2 G)
FE dofs time discretization = 240 (P1-P0 PG)

[Hec12]



MODEL ORDER REDUCTION

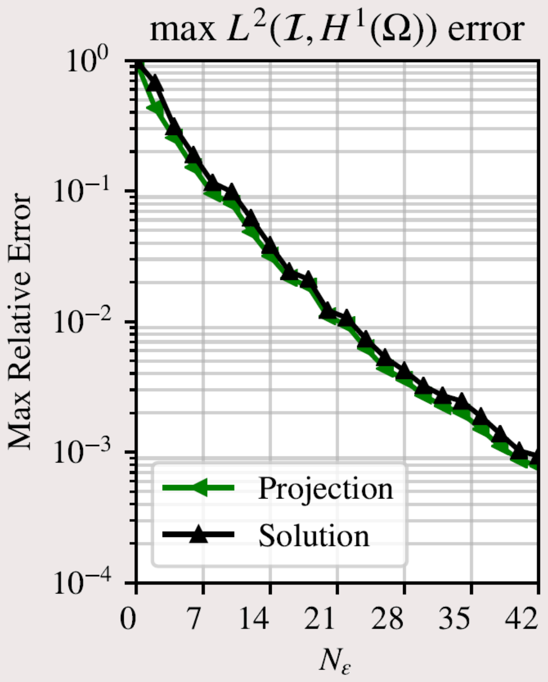
[Gre12]

considering a fine **FE discretization** as exact model

FE dofs spatial discretization = 10100 (P2-P2 G)
FE dofs time discretization = 240 (P1-P0 PG)

employing the **weak-greedy-POD** algorithm, we achieve relative error $\varepsilon < 10^{-3}$ with 42 spatial basis functions

RB dofs spatial discretization = N_ε (RB-RB G)
FE dofs time discretization = 240 (P1-P0 PG)



MODEL ORDER REDUCTION

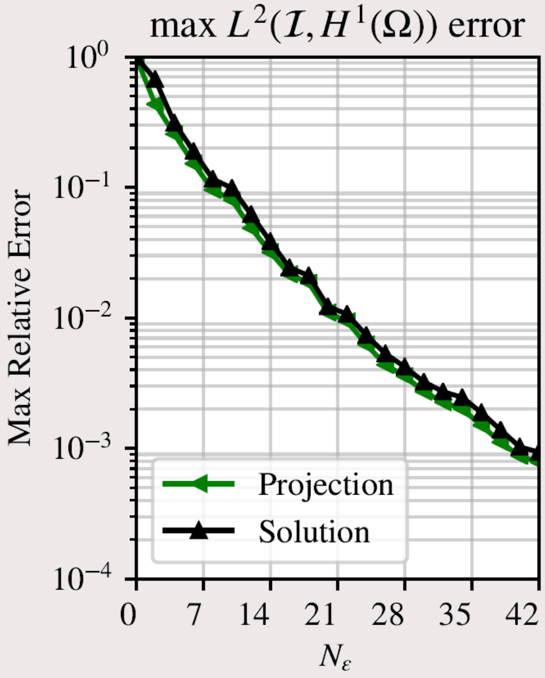
considering a fine **FE discretization** as exact model

FE dofs spatial discretization = 10100 (P2-P2 G)
FE dofs time discretization = 240 (P1-P0 PG)

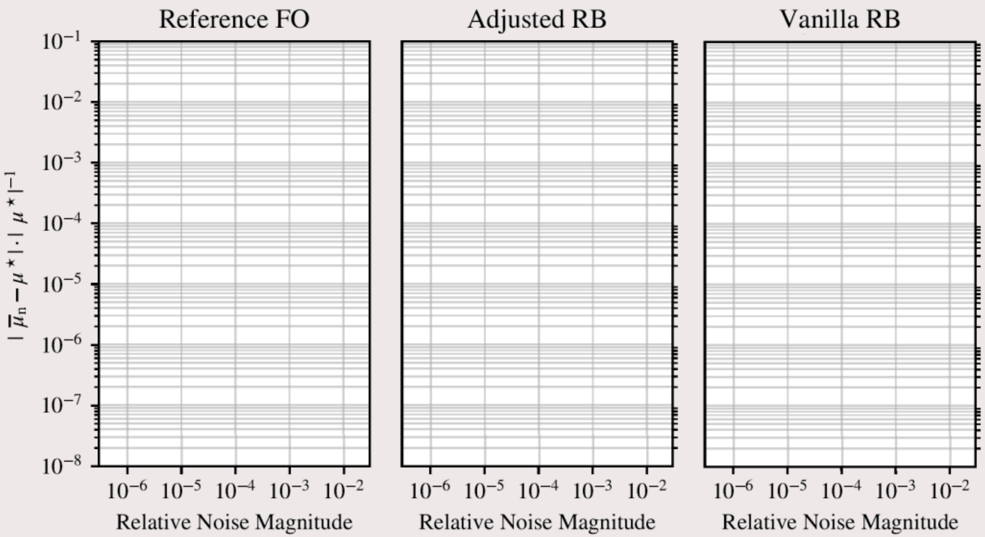
employing the **weak-greedy-POD** algorithm, we achieve relative error $\varepsilon < 10^{-3}$ with 42 spatial basis functions

RB dofs spatial discretization = N_ε (RB-RB G)
FE dofs time discretization = 240 (P1-P0 PG)

training time $\sim$**2 min**, speed up $\times$ **250**



PARAMETER ESTIMATION : NOISE EFFECTS



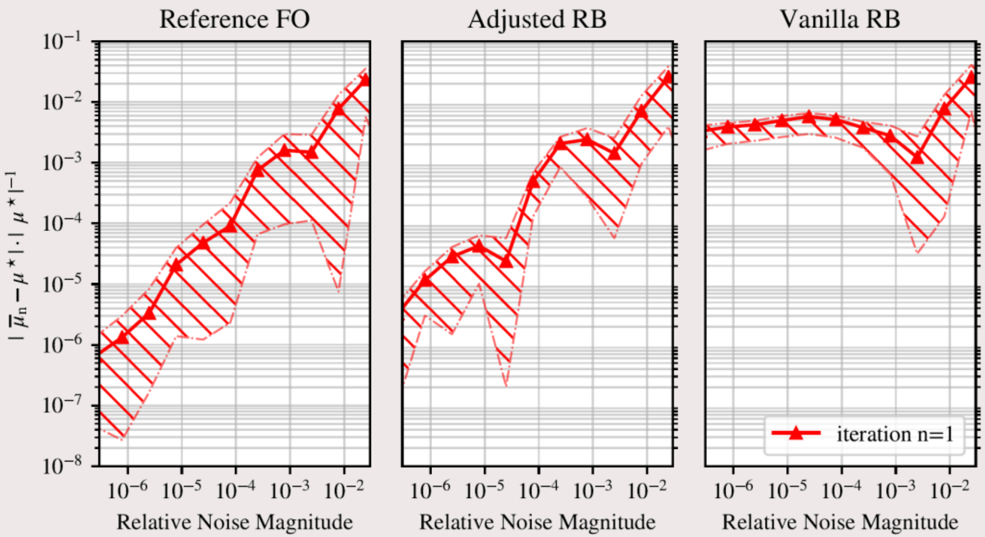
we try to estimate the $\boldsymbol{\mu}^\star = 1/25$ from noisy observations of $u(\boldsymbol{\mu}^\star)$

we consider different relative noise magnitudes $\lambda_{\max}^{1/2}(\Sigma)/\|\mathbf{L}u(\boldsymbol{\mu}^\star)\|_\infty$

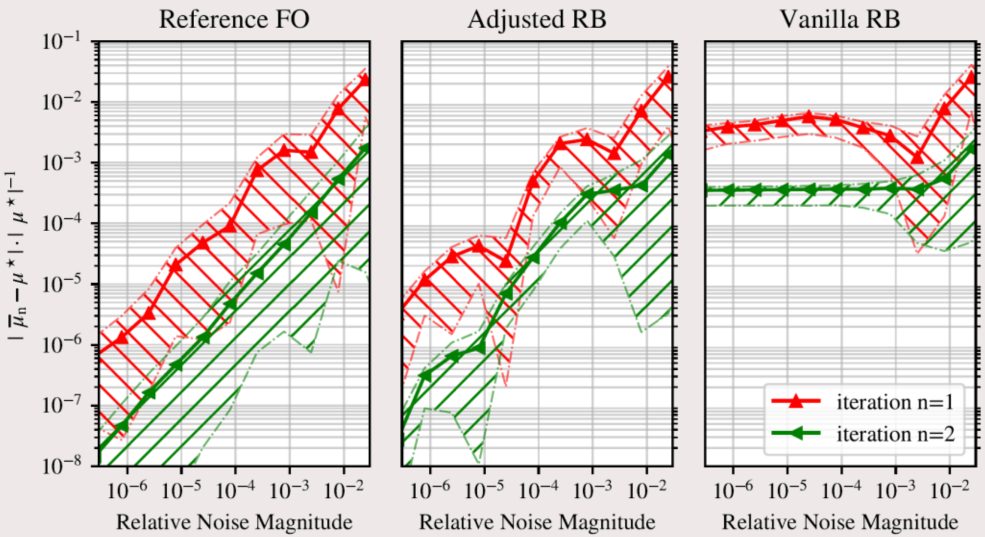
we sample ensembles of size $J = 40$ from the prior $\pi_0 = U(1/10, 1/50)$

we replicate the analysis 64 times for each noise level

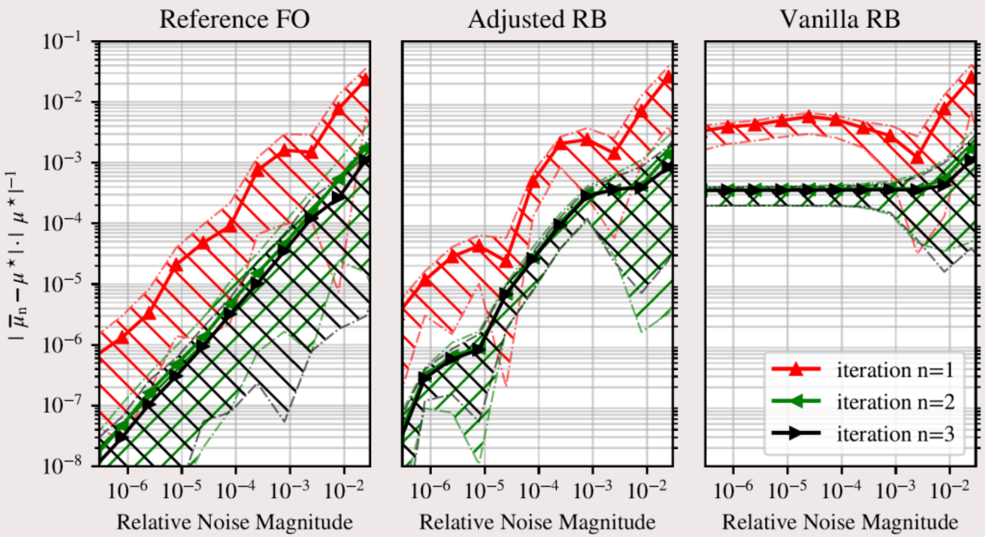
PARAMETER ESTIMATION : NOISE EFFECTS



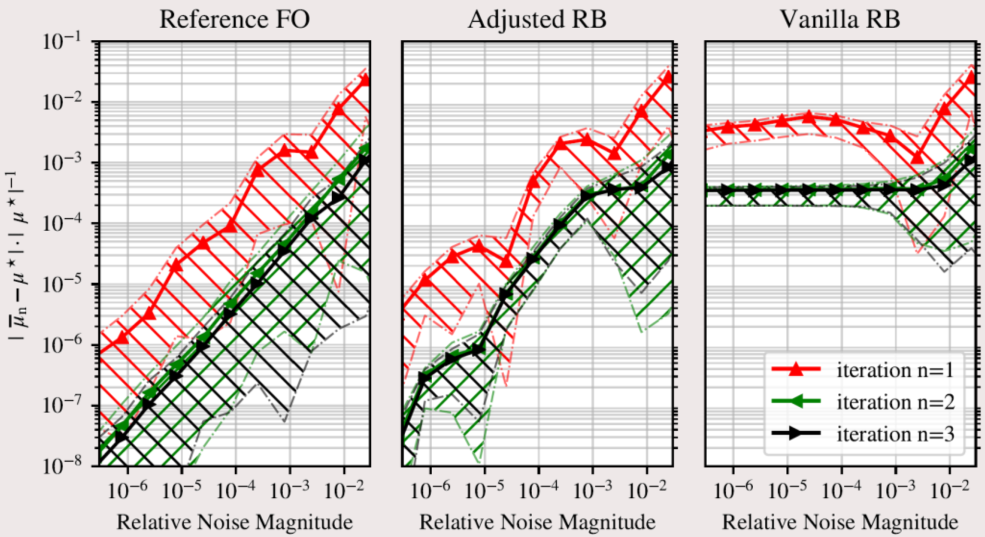
PARAMETER ESTIMATION : NOISE EFFECTS



PARAMETER ESTIMATION : NOISE EFFECTS



PARAMETER ESTIMATION : NOISE EFFECTS



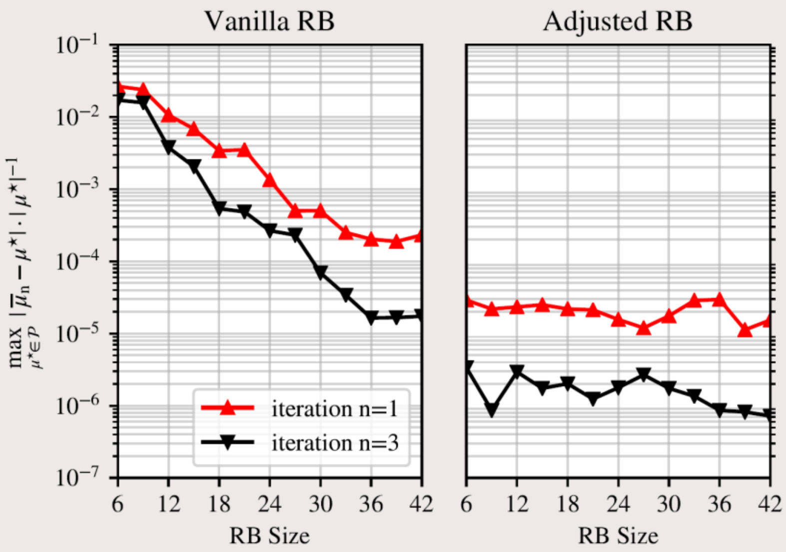
results show a linear convergence when the exact FO model is employed

the error stagnates when the model bias is not corrected in the RB-EnKM

the adjusted RB-EnKM shows an error decay comparable with the FO one

the cost of the RB-EnKM is just $\sim 4\%$ of the cost of the standard EnKM

PARAMETER ESTIMATION : REDUCED BASIS SIZE



when the measurements bias is not corrected, the relative error is strictly dependent on the RB model accuracy

with the bias correction, the performances of the method are made independent on the RB size (at least for this problem)

OUTLINE

CONCLUSIONS

SUMMARY :

- we introduced Reduced Basis solvers to improve the EnKM efficiency
- we adjusted the method to guarantee the robustness to model-biases
- we tested the method both on linear and non-linear 2D problems

OUTLOOK :

- the bias correction could be updated as the particles distribution evolves
- the approach could be extended to synchronous data assimilation problems

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THANKS FOR YOUR ATTENTION!

QUESTION TIME