Certified Reduced Basis Methods for Variational Data Assimilation

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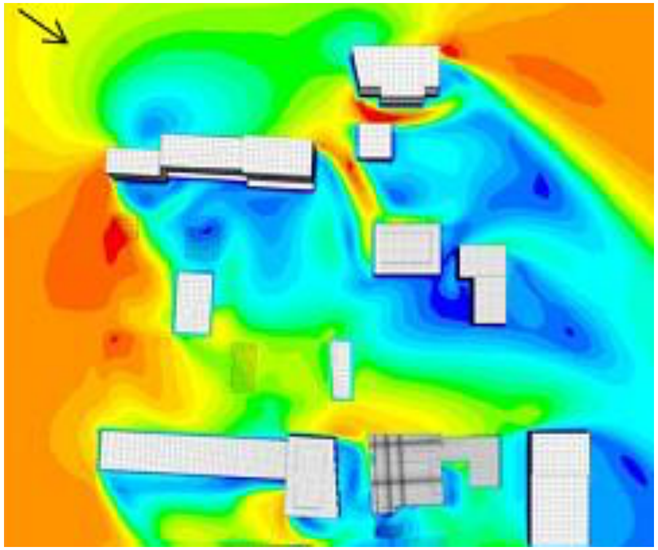
EXC-2023 : Clusters of Excellence - Internet of Production

IGPM : Institut für Geometrie und Praktische Mathematik - RWTH-Aachen

PHS : The Future of Scientific Computing: Predictive Hierarchical Simulation - Helmholtz association

AICES : Aachen Institute for Advanced Study in Computational Engineering Science - RWTH Aachen

MOTIVATION FOR SPACE-TIME DATA ASSIMILATION



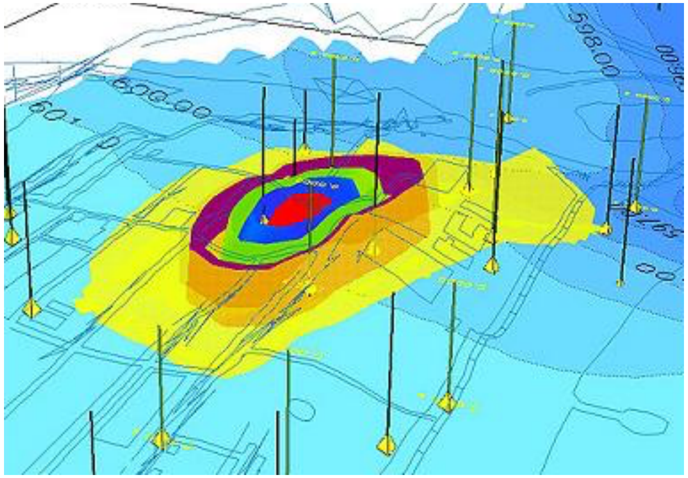
Picture from "CFD Simulation of Pollutant Gas Dispersion in Downtown Montreal, Canada", Z. Huijbregts et al., TU/e

Meteorology

- Weather forecasting
- Air pollution studies
- …

Hydrology

- Groundwater management
- Transport of contaminants
- …

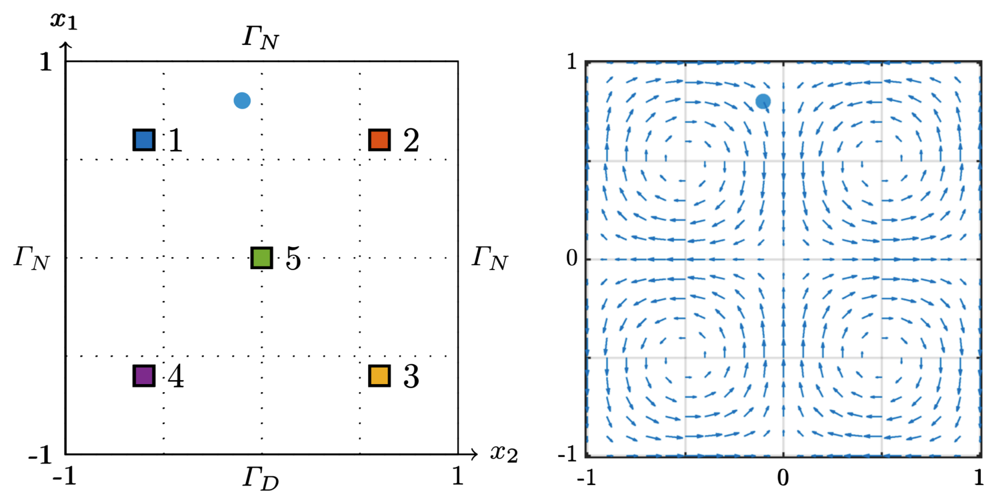


Picture from GroundwaterSoftware.com

4D-VAR CHALLENGES

4D-VAR goals:

- State forecasting
- IC/BC estimation
- Sensor location



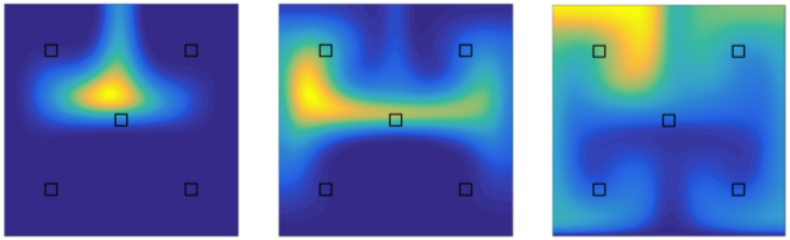
M. Kärcher, S. Boyaval, M. Grepl, K. Veroy: “Reduced basis approximation and a posteriori error bounds for 4D-VAR data assimilation”

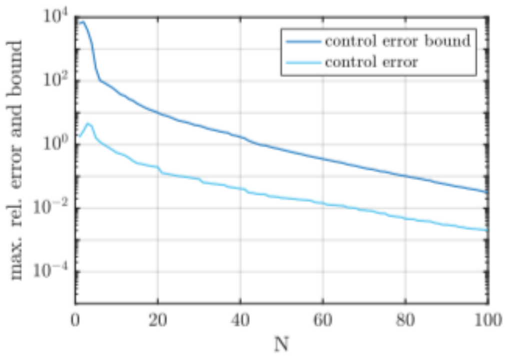
4D-VAR developments:

- Model Order Reduction [Already in early ’00, e.g. IM Navon et al.]
- A posteriori Error Bounds [M Kärcher et al. 2018]
- Optimal Criteria for Sensor Location [N Aretz-Nellesen et al. 2019]

ONGOING OUTCOMES

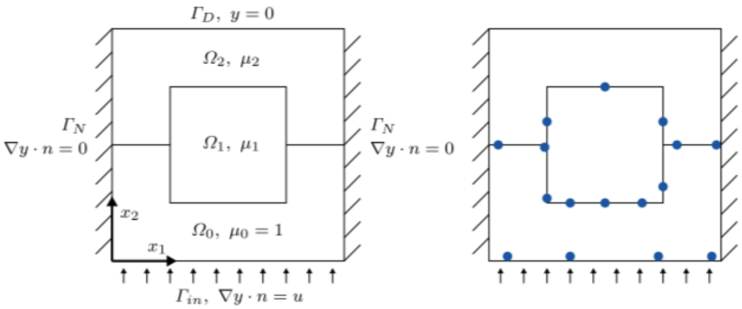
ROM-4D-VAR Results:

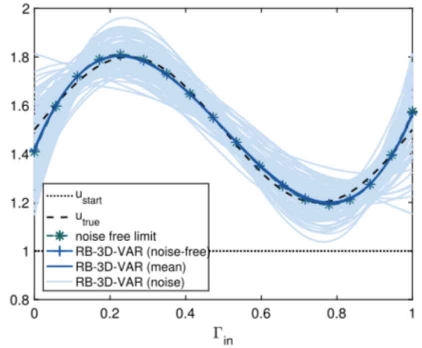




[M. Kärcher et al. 2018]

ROM-3D-VAR Results:





[N. Aretz-Nellesen et al. 2019]

STRONG 4D-VAR

$$\min_{u \in \mathcal{U}} \frac{1}{2} \|u - u_b\|^2_{\mathcal{U}} + \frac{\lambda}{2} \sum_{k=1}^{K} ||\mathcal{H} y^k(t) - y_d^k(t)||_{\mathcal{Y}} \, \Delta t$$

$$s.t. \quad y^k = \mathcal{M} y^{k-1} \; ; \quad y^0 = u$$

model

← perturbation (1st step OCP)

$\mathcal{U}$	Background error covariance	u	Initial condition
$\mathcal{Y}$	Observational error covariance	u_b	Prior estimation
$\mathcal{M}$	Evolution model (parametric)	y^k	State at t_k
$\mathcal{H}$	Observator	y_d^k	Experimental data at t_k

WEAK-CONSTRAINT 4D-VAR (MODIFIED)

$$\min_{\substack{u \in \mathcal{U} \\ b \in \mathcal{B}}} \frac{1}{2}||u - u_b||^2_{\mathcal{U}} + \frac{1}{2}\int_0^T ||b(t)||^2_{\mathcal{B}} dt + \frac{\lambda}{2}\int_0^T ||\Pi_\tau y(t) - y_d(t)||^2_{\mathcal{Y}} dt$$

$$s.t. \quad \begin{cases} (\dot{y}, v) + a_\mu(y, v) = f_\mu(v) + (b, v) \\ (y(0), v) = (u, v) \end{cases} \quad \begin{matrix} \equiv \quad My = f \\ \equiv \quad y^0 = u \end{matrix}$$

both perturbed
(continuous time OCP)

$b \in \mathcal{B}$: model perturbation

$\Pi_\tau : \mathcal{Y} \to \mathcal{T}$: projection on the sensors space (to be built)

$a_\mu(\cdot, \cdot) = (A_\mu \cdot, \cdot)$: spatial operator

LAGRANGIAN

$$\mathcal{L}(y,p,u,b) = \frac{1}{2}||u-u_b||^2_{\mathcal{U}} + \frac{T}{2}||b||^2_{\mathcal{B}} + \frac{\lambda}{2}\int_0^T ||\Pi_\tau y - y_d||^2_{\mathcal{Y}} dt$$

$$+ \int_0^T (\dot{y},p) + a_\mu(y,p) - f_\mu(p) - (b,p)\, dt$$

The problem can be reduced now:

CONTROL: $\mathcal{B} \rightarrow \mathcal{B}_R$ (forcing term RB)
$\mathcal{U} \rightarrow \mathcal{U}_R$ (initial condition RB)
} commonly low dimensional

STATE/ ADJOINT: $\mathcal{Y} \rightarrow \mathcal{Y}_R = \mathcal{Y}_y + \mathcal{Y}_p$
} construction of these RB spaces should be discussed in detail

Or after the optimization…

FULL ORDER OPTIMALITY CONDITION

(1) $$\frac{\partial \mathcal{L}}{\partial p} : (\dot{y}, \psi) + a_\mu \, (y, \psi) = (b, \psi) + f_\mu(\psi)$$ Forward Equation

(2) $$\frac{\partial \mathcal{L}}{\partial y} : (\varphi, \dot{p}) - a_\mu \, (\varphi, p) = \lambda \, (\Pi_\tau y - y_d, \Pi_\tau \varphi)$$ Adjoint Equation

(3) $$\frac{\partial \mathcal{L}}{\partial u} : (\phi, p(0)) = (u - u_b, \phi)$$ Initial/Final Condition

(4) $$\frac{\partial \mathcal{L}}{\partial b} : \int_0^T (\varphi, p) \; dt = \int_0^T (b, \varphi) \, dt$$ Forcing Term Condition

DISCRETISED (P0) AND REDUCED OPTIMALITY CONDITIONS

(1) $$\frac{\partial \mathcal{L}}{\partial p_R^k} : \left(\frac{y_R^k - y_R^{k-1}}{\Delta t}, \psi \right) + a_\mu \left(y_R^k, \psi \right) = \left(b_R, \psi \right) + f_\mu^k(\psi) \qquad \forall \psi \in \mathcal{Y}_R$$

(2) $$\frac{\partial \mathcal{L}}{\partial y_R^k} : \left(\varphi, \frac{p_R^k - p_R^{k-1}}{\Delta t} \right) - a_\mu \left(\varphi, p_R^{k-1} \right) = \lambda \left(\Pi_\tau y_R^{k-1} - y_d^{k-1}, \Pi_\tau \varphi \right) \quad \forall \varphi \in \mathcal{Y}_R$$

(3) $$\frac{\partial \mathcal{L}}{\partial u_R} : \left(\phi, p_R^1 \right) = \left(u_R - u_b, \phi \right) \qquad \forall \phi \in \mathcal{U}_R$$

(4) $$\frac{\partial \mathcal{L}}{\partial b_R} : \left(\eta, \sum_{k=1}^{K} p_R^k \frac{\Delta t}{T} \right) = \left(b_R, \eta \right) \quad \forall \eta \in \mathcal{B}_R$$

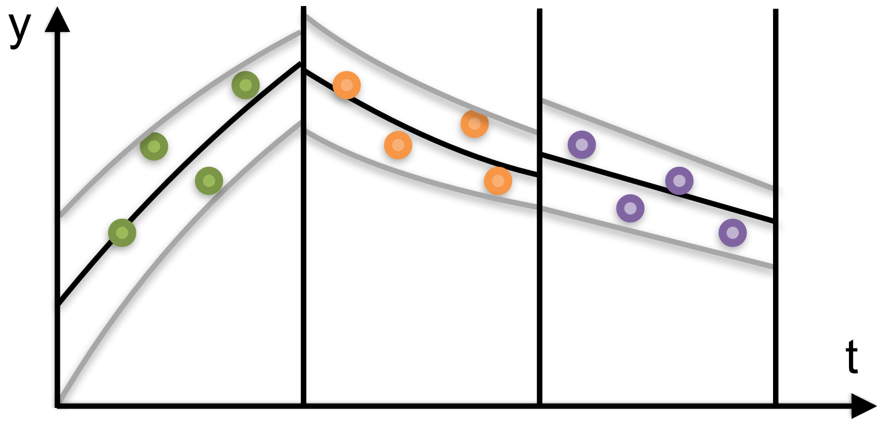
(1) Forward Equation

(2) Adjoint Equation

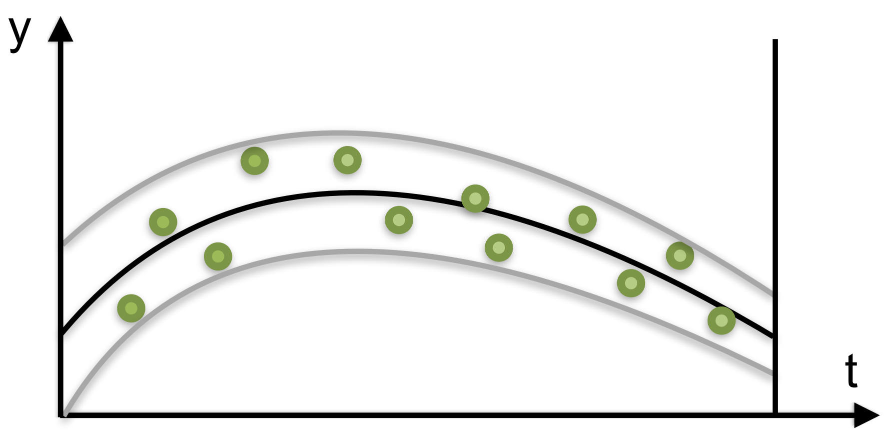
(3) Initial/Final Condition

(4) Forcing Term Condition

ADVANTAGES OF REDUCED BASIS



Too expensive to treat all experimental data in a single assimilation window using a full order model



Using RB approach the problem becomes smaller and fast, but we need to guarantee:

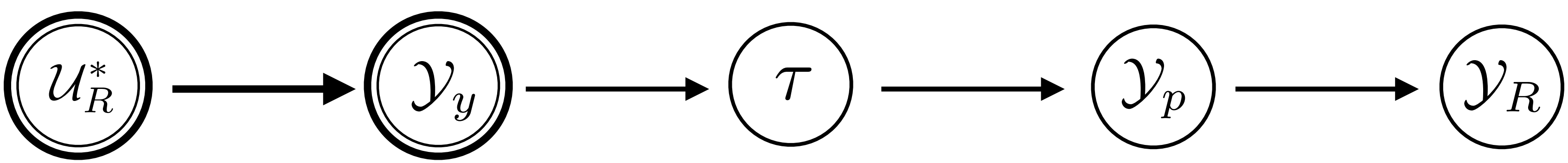
- stability
- well-posedness
- unbiased approx.

RB SPACE CONSTRUCTION AND SENSORS SELECTION

- $\left.\begin{array}{l} \mathcal{U}_R : \text{IC Space} \equiv \mathcal{U} \\ \mathcal{B}_R : \text{Par. Space} \equiv \mathcal{B} \end{array}\right\}$ assumed low dimensional

- $\mathcal{Y}_y$: greedy-POD $\left(y_\mu^{u,b}(t)\right)$: $y_\mu^{u,b}(t)$ forward solutions parametrised in u_R, b_R

$$\begin{cases} (y^k - y^{k-1}, \psi) + \Delta t \, a_\mu(y^k, \psi) = (b_R, \psi) + f_\mu(\psi) & \forall \psi \in \mathcal{Y} \\ (y^0, \psi) = (u_R, \psi) & u_R \in \mathcal{U}_R, b_R \in \mathcal{B}_R \end{cases}$$



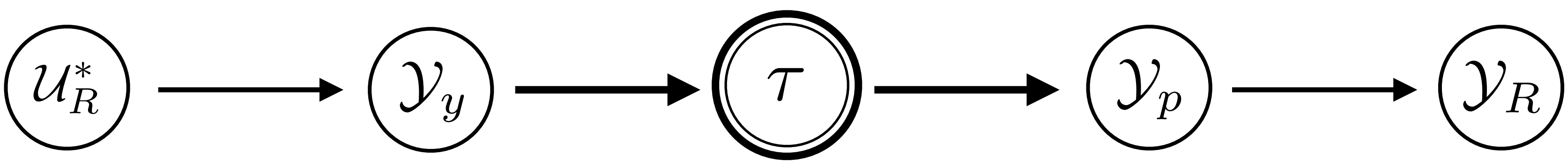
SENSORS SELECTION: MANY OPTIONS

(a) Measurements over time interval: $\tau_l^i(\cdot) = \int_{t_i}^{t_i+\Delta t_i} h_l(\cdot)\, dt \;\rightarrow\; \tau_l^i \in \mathcal{X}'$

(b) Measurements at a give time: $\tau_l^i(\cdot) = \delta(t - t_i) * h_l(\cdot) \;\rightarrow\; \tau_l^i \in \mathcal{X}'$

(c) Measurement in continuous time: $\tau_l^{(t)}(\cdot) = h_l(\cdot) \;\rightarrow\; \tau_l^{(t)} \in \mathcal{Y}'$

$$\text{where } \mathcal{X}' \text{ is dual to } \mathcal{X} = L_2(0,T;\mathcal{Y}) \cap H_1(0,T;\mathcal{Y}')$$



SENSORS SELECTION - GREEDY OMP (C)

Let's define:

$$\beta_{\mathcal{T}}(\mu) = \inf_{\substack{u \in \mathcal{U}_R \\ b \in \mathcal{B}_R}} \inf_{t \in I} \sup_{\tau \in \mathcal{Y}'} \frac{\tau^{(t)}(y_{\mu}^{u,b}(t))}{||\tau^{(t)}||_{\mathcal{Y}'} \cdot ||y_{\mu}^{u,b}(t)||_{\mathcal{Y}}} \longrightarrow \beta = \inf_{\mu \in \Xi_T} \beta_{\mathcal{T}}(\mu)$$

We use the Greedy-OMP[1] (Orthogonal Matching Pursuit) to select sensors out of a dictionary, which maximise this β coefficient. This is an extension to 4D-VAR of what has already been done for 3D-VAR[2]

[1] P. Binev, A. Cohen, O. Mula, J. Nichols : "Greedy algorithms for Optimal Measurements Selection in State"

[2] N. Aretz-Nellesen, M. Grepl, K. Veroy-Grepl : "3D-VAR for Parametrized Partial Differential Equations: …"

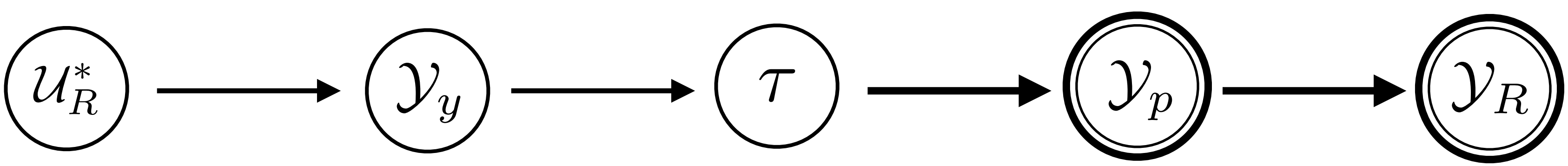
ADJOINT SPACE CONSTRUCTION

- $\mathcal{Y}_p$: greedy-POD $(p_\mu^\tau(t))$: $p_\mu^\tau(t)$ adjoint solutions parametrised in $\tau_l^{(t)}$

$$\begin{cases} (\varphi, p_R^k - p_R^{k-1}) + \Delta t \, a_\mu(\varphi, p_R^{k-1}) = \lambda \, (s_l, \Pi_\tau \varphi) & \forall \varphi \in \mathcal{Y}_R \\ (\varphi, p_R^K) = 0 & s_l \in \mathcal{T} \end{cases}$$

$$\text{where} \quad s_l \in \mathcal{Y} \; : \; \tau_l^{(t)}(\psi) = y(s_l, \psi)_{\mathcal{X}} \quad \forall \psi \in \mathcal{X}$$

- $\mathcal{Y}_R = \mathcal{Y}_y \cup \mathcal{Y}_p$



ITERATIVE SCHEME

while :

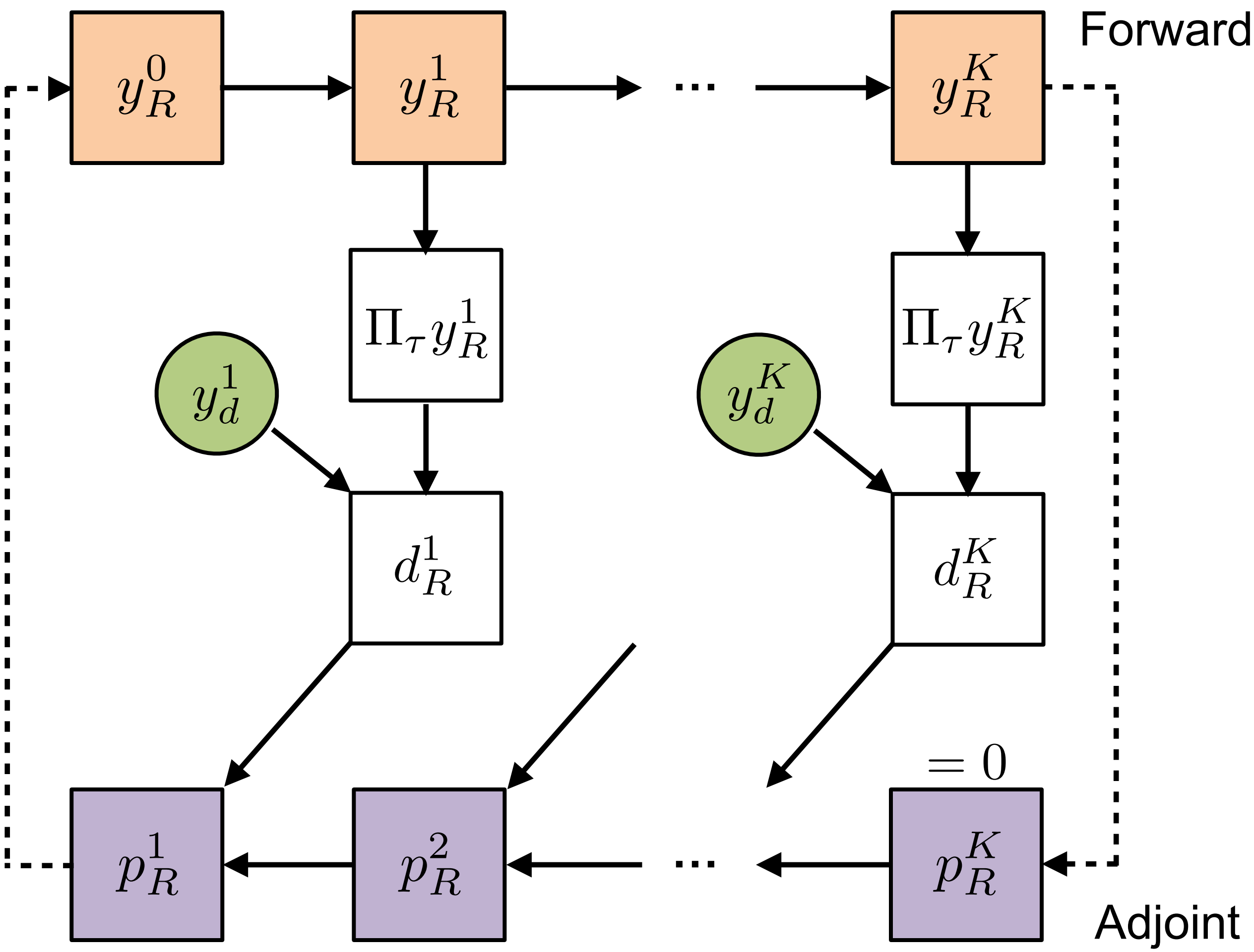
$$\|\tilde{u}_R - u_R\|_{\mathcal{U}} > \delta_u$$

$$\|\tilde{b}_R - b_R\|_{\mathcal{B}} > \delta_b$$

do :

$$b_R = \frac{1}{T}\sum_{k=1}^{K} p_R^k \Delta t$$

$$y_R^0 = p^1 + u_b$$



SHORT TERM CHALLENGES

Theoretical:

- Developing proof of stability for Forward & Adjoint Problem
- Developing a-posteriori Error Bounds for different space-time schemes

Implementation:

- Modelling space-time Sensors
- Developing space-time Orthogonal Matching Pursuit
- Developing space-time CG-P1 (Crank-Nicholson) discretisation

THANK YOU FOR YOUR ATTENTION

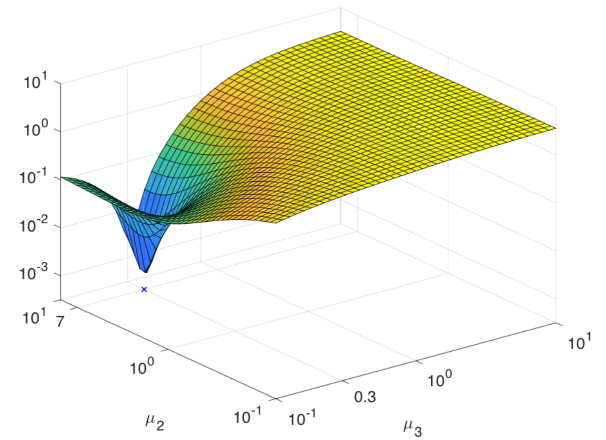
4D-VAR (μ): PARAMETER ESTIMATION

$$\min_{\mu\in\mathcal{D}} \min_{\substack{u_R\in\mathcal{U}_R\\ b_R\in\mathcal{B}_R}} \frac{1}{2}\|u_R(\mu)-u_b\|^2_{\mathcal{U}} + \frac{1}{2}\|b_R(\mu)\|^2_{\mathcal{B}} + \frac{\lambda}{2}\sum_{k=1}^{K}\|\underbrace{\Pi_\tau y_R^k(\mu)-y_d^k}_{d_R^k(\mu)}\|^2_{\mathcal{Y}}\,\Delta t$$

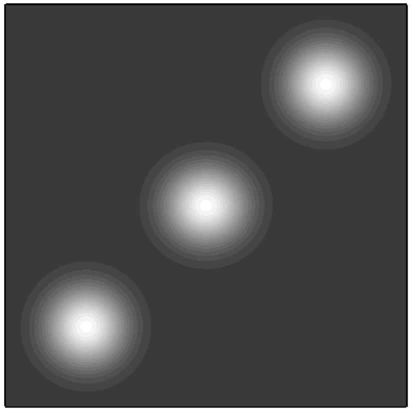
Two levels optimisation problem. It can be quite expensive to solve, hence we provide surrogate cost functions J^λ for the parameters estimation:

$$J_1^\lambda = \frac{\lambda}{2}\sum_{k=1}^{K}\|d_R^k(\mu)\|^2_{\mathcal{Y}}$$

$$J_2^\lambda = \frac{\lambda}{2}\sum_{k=1}^{K}\|d_R^k(\mu)\|^2_{\mathcal{Y}} + \frac{1}{2}\|u_R(\mu)-u_b\|^2_{\mathcal{U}}$$

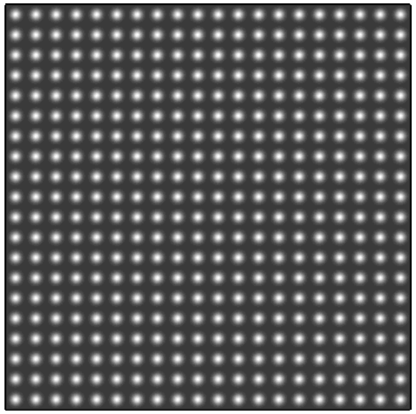


PRELIMINARY RESULTS



Model:

- 3 Possible initial conditions
- Known convection field
- Diffusivity $\mu \in [10, 50]$
- Dictionary of sensors on a regular grid



Assumptions:

- Exact position of sensors
- Uncertainty only due to IC and Noise
- No model bias