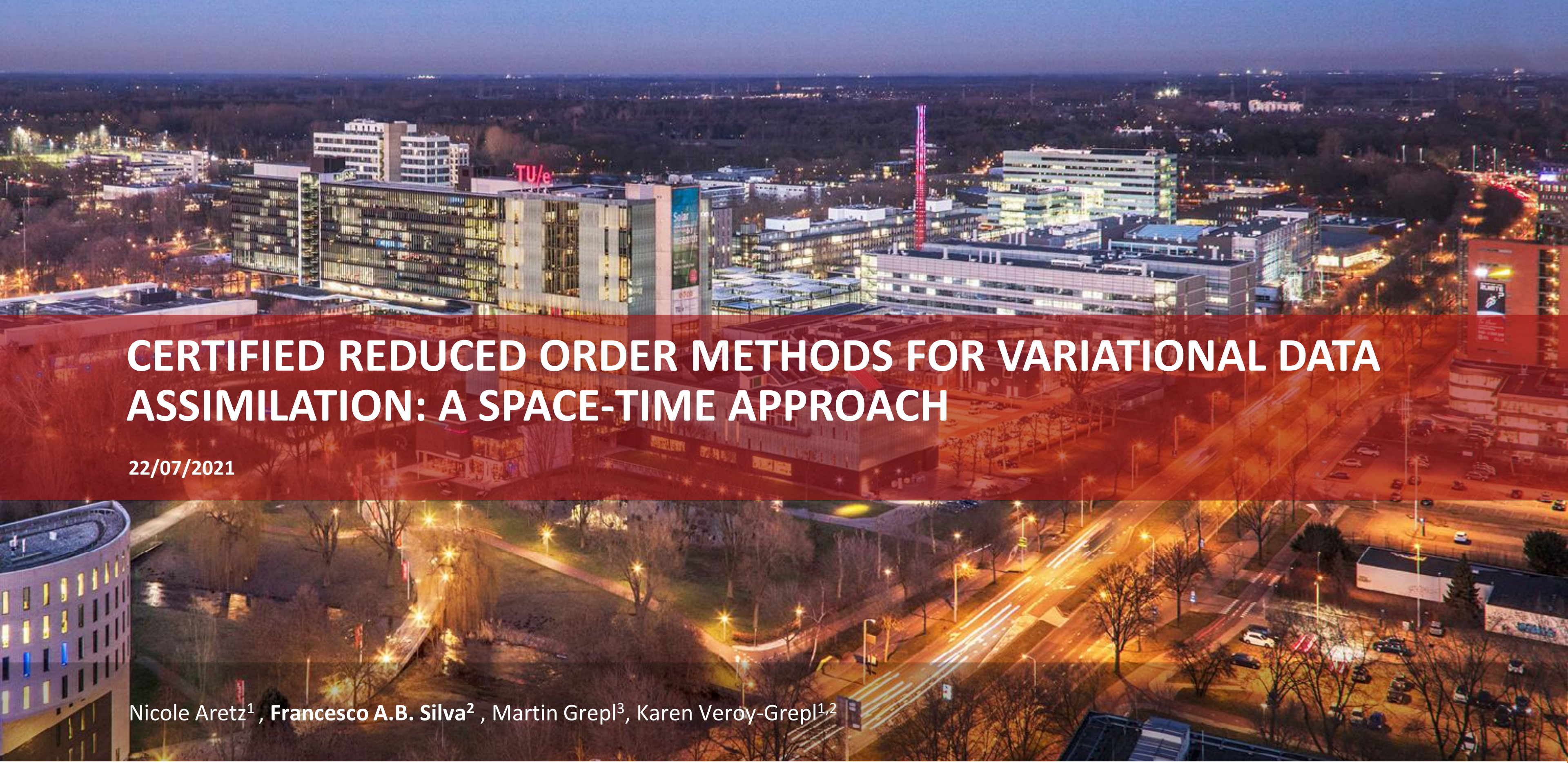

CERTIFIED REDUCED ORDER METHODS FOR VARIATIONAL DATA ASSIMILATION: A SPACE-TIME APPROACH

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DATA ASSIMILATION

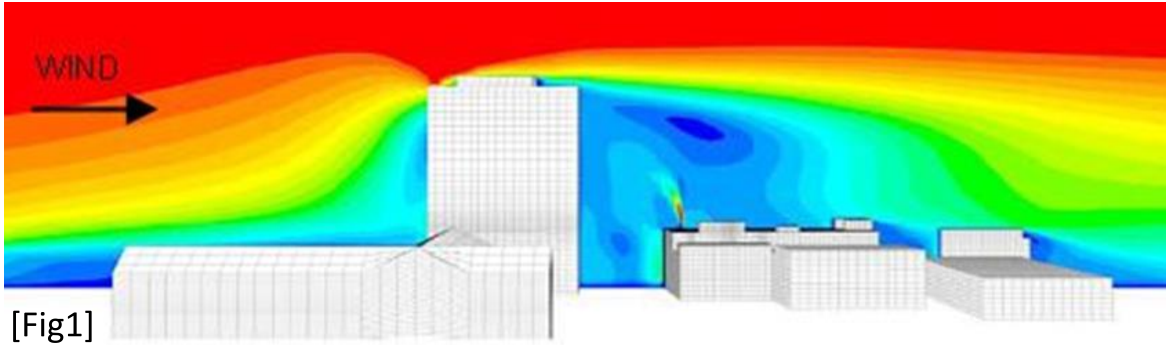
MOTIVATION FOR DATA ASSIMILATION

METEREOLOGY

- Weather forecast
- Air pollution studies
- …

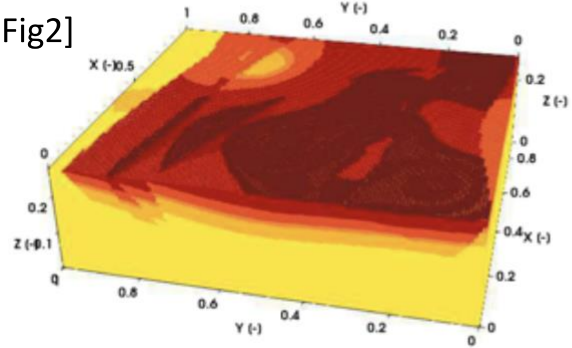
HYDROLOGY

- Ground water management
- Transport of contaminants
- …



[Fig1]

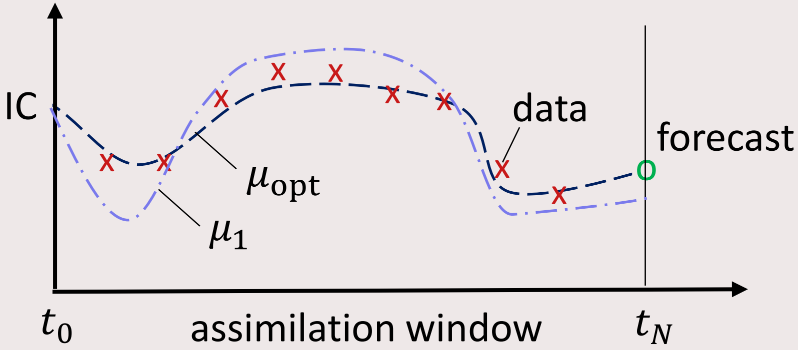
[Fig2]



VARIATIONAL DATA ASSIMILATION

GOAL OF THE METHOD

- State forecasting
- Parameter estimation
- IC/BC estimation



STATE OF THE ART

- Reduced Order Modelling [D. N. Daescu et al. 2006]
- A posteriori error bounds [M. Kärcher et al. 2018]
- Optimal sensor location [P. Binev et al 2019]

VARIATIONAL DATA ASSIMILATION – WHAT DO WE NEED?

ON THE MODEL SIDE

- Model of the physical system ⟶ Parametric PDE : $A_\mu x = b_\mu$
- A Data Assimilation scheme ⟶ 4D-VAR
- Model of the observation process ⟶ Linear functional : $Lx = m$

ON THE EXPERIMENTAL SIDE

- Measurements ⟶ Experimental data : $d = Lx^{\text{TRUE}} + \epsilon$
- Noise properties ⟶ Noise : $\epsilon \sim N(0, \Sigma)$

STRONG 4D-VAR – AN OPTIMAL CONTROL PROBLEM

$$\min_{u \in \mathcal{U}} \mathcal{J}(u \mid \mu, d) := \boxed{\frac{1}{2}\|Lx - d\|_{\mathcal{Z}}^2} + \boxed{\frac{\lambda}{2}\|u\|_{\mathcal{U}}^2} \quad s.t. \quad \boxed{a_\mu(x,\psi) = f_\mu^{\mathrm{bk}}(\psi) + b_\mu(u,\psi) \quad \forall \psi \in \mathcal{Y}}$$

MISFIT STABILIZATION MODEL

where:

$d \in \mathcal{Z}$: Measurements

$u \in \mathcal{U}$: Initial conditions

$x \in \mathcal{X}$: Bochner state

λ : depends on the trust we have in the prior knowledge !

we assume:

$d = Lx^{\mathrm{TRUE}} + \epsilon$ *with noise* $\epsilon \sim N(0, \Sigma)$

PARABOLIC PARAMETRIC PDEs - SPACE-TIME APPROACH

$$\dot{x}(t) + C_\mu x(t) = g_\mu(t) \quad \text{in } \mathcal{V}', \text{ a.e. } t \in I := [0,T]$$
$$x(0) = u \quad \text{in } \mathcal{H}$$

from which the variational formulation:

$$\int_I \langle \dot{x}(t) + C_\mu x(t), \eta(t) \rangle_{\mathcal{H}} \, dt = \int_I \langle g_\mu(t), \eta(t) \rangle_{\mathcal{H}} dt \qquad \forall \ \boxed{\eta(t)} \in \boxed{L^2(I, \mathcal{V})}$$
$$\langle x(0), \xi \rangle_{\mathcal{H}} = \langle u, \xi \rangle_{\mathcal{H}} \qquad \forall \ \boxed{\xi} \in \boxed{\mathcal{H}}$$

ψ $\quad$ $\mathcal{Y}$

that can be rewritten as:

$$\boxed{a_\mu(x, \psi) = f_\mu^{\text{bk}}(\psi) + b_\mu(u, \psi) \quad \forall \psi \in \mathcal{Y}} \qquad x \in \mathcal{X} := L^2(I, \mathcal{V}) \cap H^1(I, \mathcal{V}'), \ u \in \mathcal{U} \subset \mathcal{H}$$

SPACE-TIME WEAK MODEL

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[K. Urban, A. Patera]

SPACE-TIME DISCRETIZATION

let’s consider a P2-P2 discretization in space and P1-P0 in time

$$x(t) = \sum_{k=0}^{K} \boldsymbol{\sigma_k(t)} x_k$$

$$\mathrm{p}(t) = \sum_{k=0}^{K} \boldsymbol{\tau_k(t)}\, p_{k,i}$$

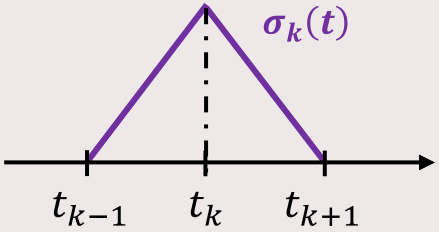
$$\longrightarrow$$

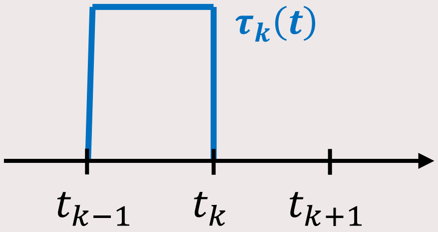
$$\langle x_k - x_{k-1}, p_{k,i} \rangle_{\mathcal{H}} + \frac{\Delta t}{2} c_\mu(x_k + x_{k-1}, p_{k,i}) = \int_{I_k} \langle g_\mu, p_{k,i} \rangle_{\mathcal{H}} dt$$

$$(x_0, \xi)_{\mathcal{H}} = (u, \xi)_{\mathcal{H}}$$

with x_k, x_{k-1} and $\eta_{k,i} \in \mathbb{P}^2$

and $c_\mu(x, \eta) = \langle C_\mu x, \eta \rangle_{\mathcal{H}}$





DISCRETE LAGRANGE OPTIMIZATION

$$\mathcal{L}(u, x, p \mid \mu, d) = \frac{1}{2}\|Lx - d\|_{\mathcal{Z}}^2 + \frac{\lambda}{2}\left\|u - u^{bk}\right\|_{\mathcal{U}}^2 + \int_I \langle \dot{x} + C_\mu x - g_\mu, p\rangle_{\mathcal{H}} dt + \langle x_0^R - u, p_0^R\rangle_{\mathcal{H}}$$

a first order optimality condition can be easily derived imposing $\delta\mathcal{L} = 0$:

$$\begin{cases} \langle x_k - x_{k-1}, \eta\rangle_{\mathcal{H}} + \frac{\Delta t}{2} c_\mu(x_k + x_{k-1}, \eta) = \int_{I_k} \langle g_\mu, \eta\rangle_{\mathcal{H}} dt & \forall\, \eta \in \mathcal{V}_{\mathrm{R}}^x \quad \text{Forward Equation} \\ \langle \varphi, p_k - p_{k+1}\rangle_{\mathcal{H}} + \frac{\Delta t}{2} c_\mu(\varphi, p_k + p_{k+1}) = \langle d - Lx, L\sigma_k \varphi\rangle_{\mathcal{Z}} & \forall \varphi \in \mathcal{V}_{\mathrm{R}}^p \quad \text{Backward Equation} \\ \lambda\langle u, \psi\rangle_{\mathcal{U}} - \langle \psi, p_0\rangle_{\mathcal{H}} = \lambda\langle u^{bk}, \psi\rangle_{\mathcal{U}} & \forall \psi \in \mathcal{U} \quad \text{Gradient Equation} \end{cases}$$

$+ \quad p_K = 0 \text{ and } x_0 = u$

MODEL ORDER REDUCTION

DISCRETE LAGRANGE OPTIMIZATION - REDUED VERSION

$$\boldsymbol{\mathcal{L}}(u, x, p \mid \mu, d) = \frac{1}{2}\left\|Lx^{\mathrm{R}} - d\right\|_{\mathcal{Z}}^{2} + \frac{\lambda}{2}\left\|u - u^{bk}\right\|_{\mathcal{U}}^{2} + \int_{I}\left\langle \dot{x}^{\mathrm{R}} + C_{\mu}x^{\mathrm{R}} - g_{\mu}, p^{\mathrm{R}}\right\rangle_{\mathcal{H}} dt + \left\langle x_{0}^{\mathrm{R}} - u, p_{0}^{\mathrm{R}}\right\rangle_{\mathcal{H}}$$

a first order optimality condition can be easily derived imposing $\delta\mathcal{L} = 0$:

$$\begin{cases} \left\langle x_k^{\mathrm{R}} - x_{k-1}^{\mathrm{R}}, \eta\right\rangle_{\mathcal{H}} + \frac{\Delta t}{2} c_{\mu}\left(x_k^{\mathrm{R}} + x_{k-1}^{\mathrm{R}}, \eta\right) = \int_{I_k}\left\langle g_{\mu}, \eta\right\rangle_{\mathcal{H}} dt & \forall\, \eta \in \mathcal{V}_{\mathrm{R}}^{x} \quad \text{Forward Equation} \\ \left\langle \varphi, p_k^{\mathrm{R}} - p_{k+1}^{\mathrm{R}}\right\rangle_{\mathcal{H}} + \frac{\Delta t}{2} c_{\mu}\left(\varphi, p_k^{\mathrm{R}} + p_{k+1}^{\mathrm{R}}\right) = \left\langle d - Lx^{\mathrm{R}}, L\sigma_k\varphi\right\rangle_{\mathcal{Z}} & \forall \varphi \in \mathcal{V}_{\mathrm{R}}^{p} \quad \text{Backward Equation} \\ \lambda\langle u, \psi\rangle_{\mathcal{U}} - \langle \psi, p_0\rangle_{\mathcal{H}} = \lambda\left\langle u^{bk}, \psi\right\rangle_{\mathcal{U}} & \forall \psi \in \mathcal{U} \quad \text{Gradient Equation} \end{cases}$$

$$+ \quad p_K^{\mathrm{R}} = 0 \quad \text{and} \quad x_0^{\mathrm{R}} = u$$

PRIMAL AND DUAL ERROR BOUND

$$\left\|x - x^{\mathrm{R}}\right\|_{\lozenge} \leq \Delta_{\mathrm{R}}^{x}(\mu) := \frac{\|r^{x}\|_{\mathcal{Y}'}}{\beta_a^{\lozenge}(\mu)}$$

$$\left\|p - p^{\mathrm{R}}\right\|_{\mathcal{Y}} \leq \Delta_{\mathrm{R}}^{p}(\mu) := \frac{\|r^{p}\|_{\lozenge'}}{\beta_a^{\lozenge}(\mu)}$$

$\longleftarrow$

$$\beta_a^{\lozenge}(\mu) = \inf_{\varphi \in \mathcal{X}} \sup_{(\nu,\xi)\in\mathcal{Y}} \frac{a_\mu(\varphi,(\nu,\xi))}{\|\varphi\|_{\lozenge}\|(\nu,\xi)\|_{\mathcal{Y}}} \geq \beta_a^{\mathrm{LB}}(\mu)$$

we introduce the residuals:

$$r^{x}(\nu,\xi) = -a_\mu\left(x^{\mathrm{R}},(\nu,\xi)\right) + \int_I \langle g_\mu, \nu\rangle_{\mathcal{H}} dt$$

$$r^{p}(\eta) \quad = -a_\mu\left(\varphi, p^{\mathrm{R}}\right) + \left\langle d - Lx^{\mathrm{R}}, L\eta\right\rangle_{\mathcal{Z}}$$

the residuals are linear functionals over the test and trial spaces $\mathcal{Y}$ and $\mathcal{X}$, their norm must be intended as a dual norm

PRIMAL AND DUAL ERROR BOUND

$$\left\| x - x^{\mathrm{R}} \right\|_{\delta} \leq \Delta_{\mathrm{R}}^{x}(\mu) \coloneqq \frac{\|r^x\|_{\mathcal{Y}'}}{\beta_a^{\delta}(\mu)} \longleftarrow \|r^x\|_{\mathcal{Y}'} = \left\| \mathcal{R}_{\mathcal{Y}} r^x \right\|_{\mathcal{Y}}$$

$$\left\| p - p^{\mathrm{R}} \right\|_{\mathcal{Y}} \leq \Delta_{\mathrm{R}}^{p}(\mu) \coloneqq \frac{\|r^p\|_{\delta'}}{\beta_a^{\delta}(\mu)} \longleftarrow \|r^p\|_{\delta'} = \|\mathcal{R}_{\delta} r^p\|_{\delta}$$

which norms are employed? $\mathcal{Y}, \mathcal{Y}'$ and… ?

$$\|(v,\xi)\|_{\mathcal{Y}}^2 = \int_I \|v\|_{\mathcal{V}}^2 dt + \|\xi\|_{\mathcal{H}}^2$$

$$\|\eta\|_{\delta}^2 = \|\eta(T)\|_{\mathcal{H}}^2 + \int_I \|\dot{\eta}\|_{\mathcal{V}'}^2 dt + \boxed{\int_I \|\bar{\eta}\|_{\mathcal{V}}^2 dt}$$

this term forbids an efficient computation $\mathcal{R}_{\delta} r^{y}$ and therefore, of the dual norm $\|r^{y}\|_{\delta'}$

PRIMAL AND DUAL ERROR BOUND

$$\left\|x - x^{\mathrm{R}}\right\|_{\mathrm{tg}} \leq \Delta_{\mathrm{R}}^{x}(\mu) := \frac{\|r^x\|_{\mathcal{Y}'}}{\beta_a^{\mathrm{tg}}(\mu)} \longleftarrow \|r^x\|_{\mathcal{Y}'} = \left\|\mathcal{R}_{\mathcal{Y}} r^x\right\|_{\mathcal{Y}}$$

$$\left\|p - p^{\mathrm{R}}\right\|_{\mathcal{Y}} \leq \Delta_{\mathrm{R}}^{p}(\mu) := \frac{\|r^p\|_{\mathrm{tg}'}}{\beta_a^{\mathrm{tg}}(\mu)} \longleftarrow \|r^p\|_{\mathrm{tg}'} = \left\|\mathcal{R}_{\mathrm{tg}} r^p\right\|_{\mathrm{tg}}$$

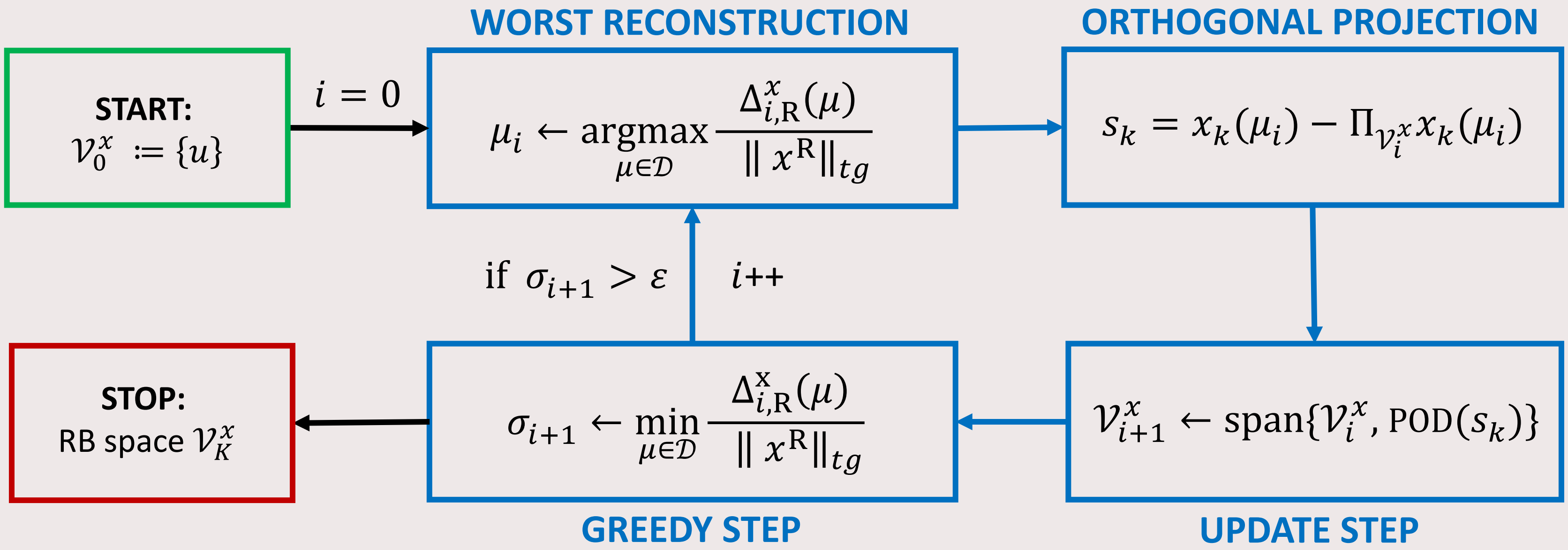
which norms are employed? $\mathcal{Y}, \mathcal{Y}'$ and $(\mathrm{tg}), (\mathrm{tg})'$!

$$\|(v,\xi)\|_{\mathcal{Y}}^2 = \int_I \|v\|_{\mathcal{V}}^2 dt + \|\xi\|_{\mathcal{H}}^2$$

$$\|\eta\|_{\mathrm{tg}}^2 = \|\eta(T)\|_{\mathcal{H}}^2 + \int_I \|\dot{\eta}\|_{\mathcal{V}'}^2 dt$$

$\mathcal{R}_{\mathrm{tg}} r^p$ can be computed efficiently online with an iterative scheme, this allows $\|r^p\|_{\mathrm{tg}'}$ to be computed

REDUCED BASIS SELECTION - GREEDY POD



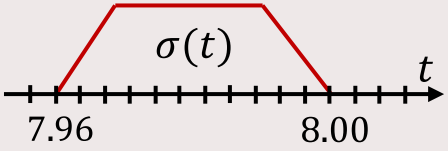
ADVECTION-DISPERSION 2D

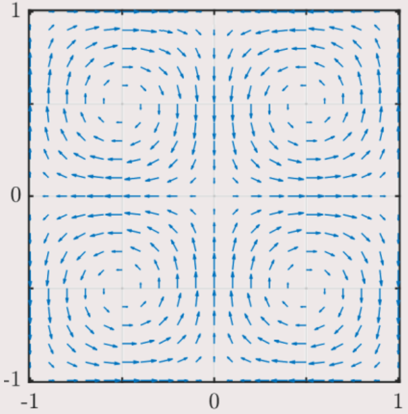
ADVECTION-DISPERSION 2D

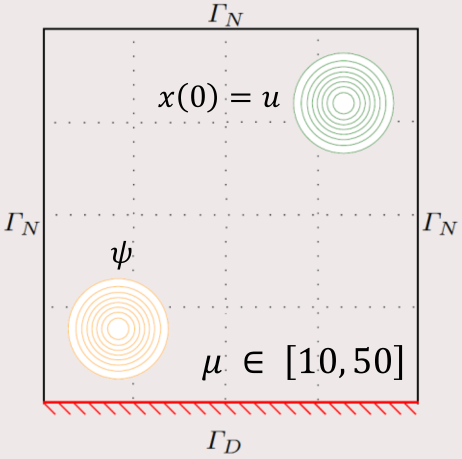
$$\frac{\partial x}{\partial t} - \frac{\Delta x(t)}{\mu} + \boldsymbol{v} \cdot \boldsymbol{\nabla} x(t) = 0 \quad \text{on } \Omega := (-1,+1)^2 \qquad \text{with} \qquad \boldsymbol{v} = \begin{bmatrix} +\sin(\pi x_1)\cos(\pi x_2) \\ -\cos(\pi x_1)\sin(\pi x_2) \end{bmatrix}$$

over the time horizon $I = (0,8)$
we define the linear functional :

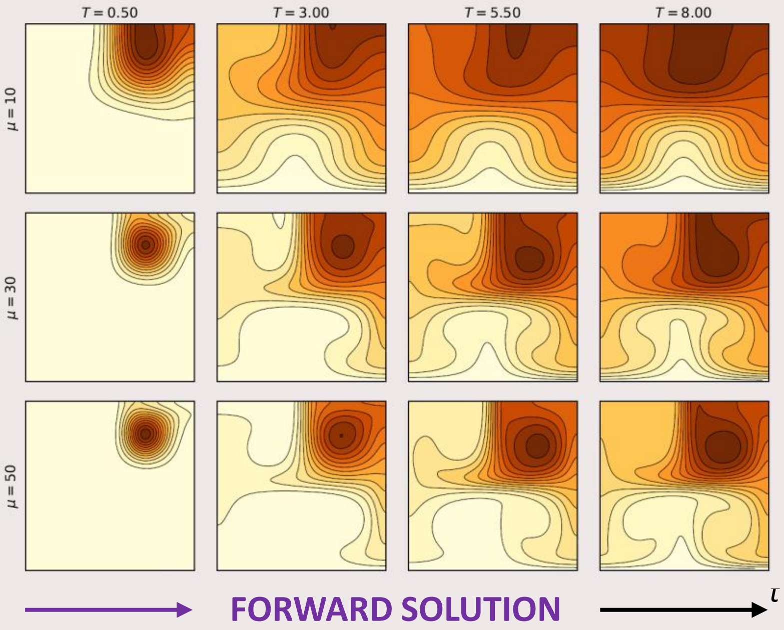
$$L\varphi(x_1,x_2,t) = \int_I \langle \varphi, \psi(x_1,x_2) \rangle_{\mathcal{H}} \sigma(t) dt$$

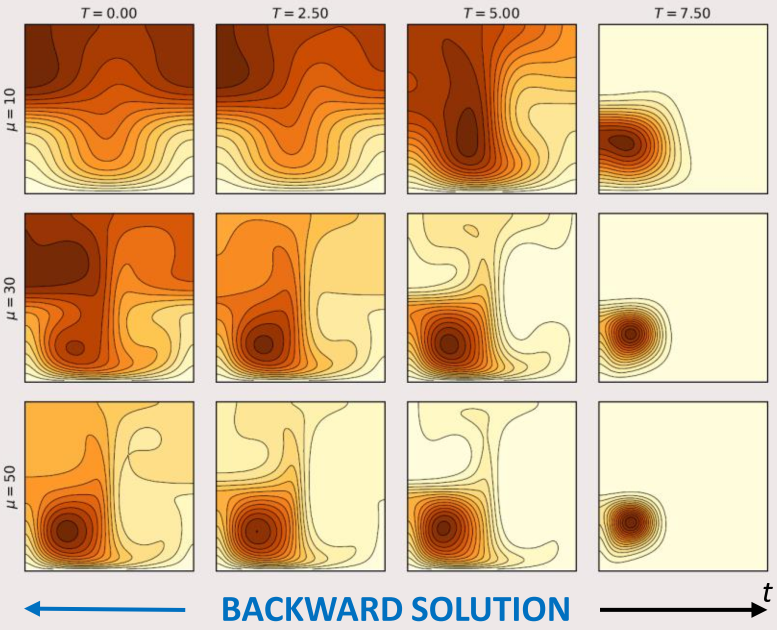






ADVECTION-DISPERSION 2D - SOLUTION SHAPE





MOR – FORWARD PROBLEM

Employing the weak-greedy-POD approach we construct a Reduced Basis space of size 48 :

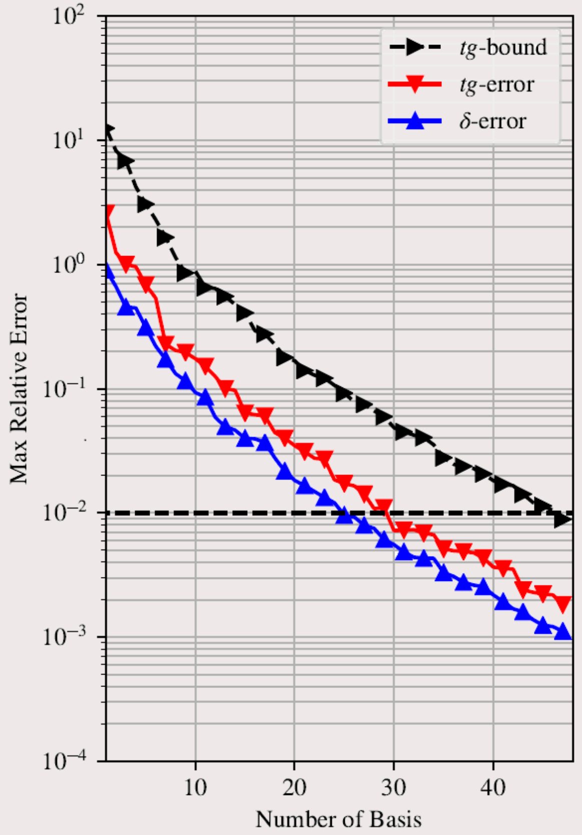
dofs spatial discretization = 10100

dofs time discretization = 801

training set size = 80

training time = 4 minutes 25 seconds

The effectivity of the bound is independent from the space dimension and doesn't exceed a factor 10



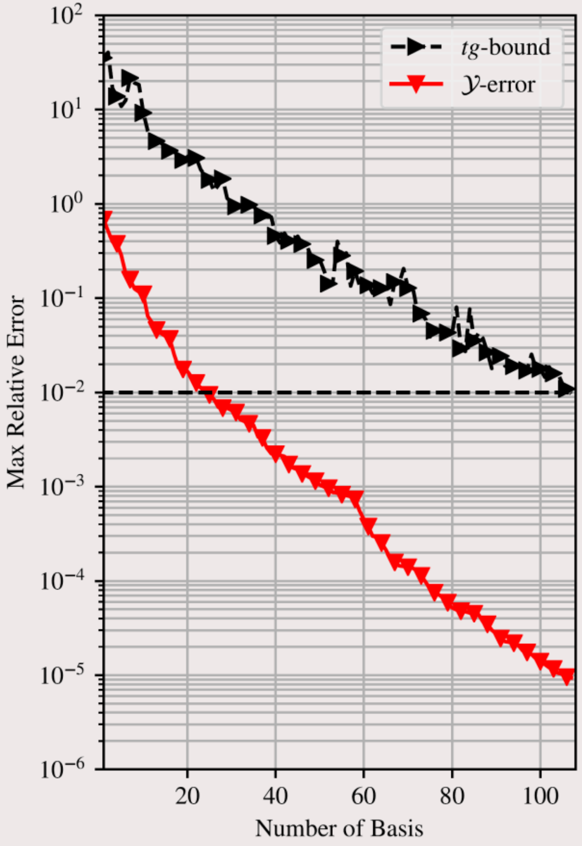
MOR – BACKWARD PROBLEM

Employing the weak-greedy-POD approach we construct a Reduced Basis space of size 108:

dofs spatial discretization = 10100
dofs time discretization = 801

training set size = 80
training time = 31 minutes 27 seconds

The effectivity of the bound depends, initially, on the space dimension and stabilizes on a factor 1000



CONCLUSIONS

WHAT HAVE WE ALREADY DONE?

- We developed an effective error bound for coercive parabolic problems
- We implemented a greedy-POD algorithm for the reduction of the problem
- We extended the greedy-OMP algorithm to space-time states [not shown]

WHAT ARE WE STILL WORKING ON?

- We are testing the 4D-VAR solver based on a Lagrange optimization scheme
- We are improving an error bound for the adjoint problem
- We are developing a gradient free scheme to solve the 4D-VAR problem

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SELECTED RELATED LITERATURE

[K. Urban, A. Patera] : An improved error bound for reduced basis approximation of linear parabolic problems

[M. Kärcher et al. 2018] : Reduced basis approximation and a-posteriori error bounds for 4D-Var data assimilation

[D. N. Daescu et al. 2006] : Efficiency of a POD-based reduced second-order adjoint model in 4D-Var data assimilation

[N. Aretz et al. 2019] : 3D-VAR for parameterized partial differential equations: a certified reduced basis approach

[Fig1] : Z. Huijbregts et al., CFD simulation of pollutant gas dispersion in downtown Montreal

[Fig2] : Denise Degen et al, Certified Reduced Basis Method in Geosciences

THANK YOU FOR YOUR ATTENTION!

QUESTION TIME!

BACK UP

ADVECTION-DIFFUSION-REACTION 1D

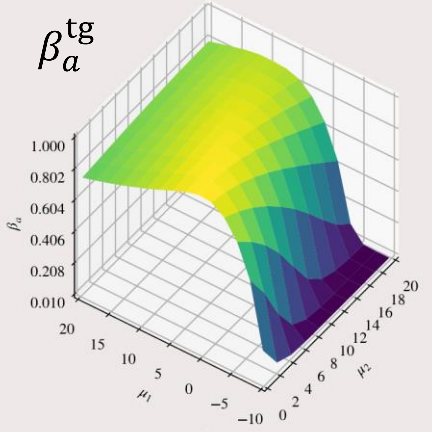
ADVECTION-DIFFUSION-REACTION 1D

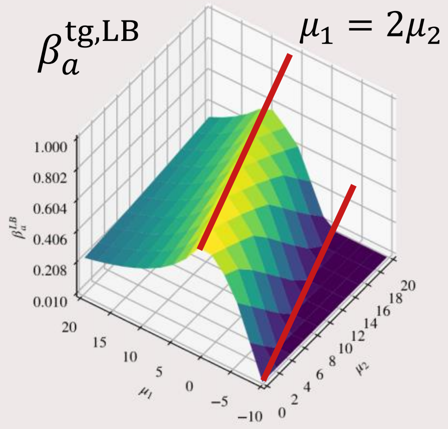
$$\frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} + \mu_1\left(x - \tfrac{1}{2}\right)\frac{\partial v}{\partial x} + \mu_2 v = 0 \qquad \text{on} \qquad \Omega := (0\,,1)$$

we use this problem to study $\beta_a^{\mathrm{tg}}(\mu)$ and its bound $\beta_a^{\mathrm{tg,LB}}(\mu)$ which applies when $c(v, w; \mu) = (\nabla v, \nabla w)_{\mathcal{H}} + \mu_2 (v, w)_{\mathcal{H}} + \mu_1 \ldots$ is coercive:

$$\alpha_c(\mu) = \inf_{v \in \mathcal{V}} \; 1 + (\mu_2 - \frac{\mu_1}{2}) \frac{\|v\|_{\mathcal{H}}^2}{\|\nabla v\|_{\mathcal{H}}^2} \geq 0$$

verified when $\mu_1 - 2\mu_2 < 2\pi^2$





ADVECTION-DIFFUSION-REACTION 1D

$$\frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} + \mu_1\left(x - \tfrac{1}{2}\right)\frac{\partial v}{\partial x} + \mu_2 v = 0$$

from this we obtain the space-time bilinear form

$$a_\mu(v,\psi) = \int_I \left(\tfrac{\partial v}{\partial t}, w\right)_{\mathcal{H}} + \mu_1\left(x\tfrac{\partial v}{\partial x} - \tfrac{1}{2}\tfrac{\partial v}{\partial x}, w\right)_{\mathcal{H}} dt + \int_I \left(\tfrac{\partial^2 v}{\partial x^2}, w\right)_{\mathcal{H}} + \mu_2 (v,w)_{\mathcal{H}}\, dt$$

inf-sup stability constant of this form on the right
the bound effectivity decreases as $\alpha_c(\mu) \to 0$