Dipartimento di Scienze Matematiche G. L. Lagrange

Optimization problems governed by PDEs under the influence of random variables

Maria Strazzullo

Department of mathematical Sciences, Politecnico of Turin

Politecnico di Torino

Power of Diversity in Uncertainty Quantification

Outline, Tools and Collaborators

Outline

1. Problem Formulation
2. Weighted Proper Orthogonal Decomposition (w-POD) approach
3. Numerical Results

Collaborators

- Francesco Ballarin, Gianluigi Rozza
- Giuseppe Carere, Fabio Zoccolan

Tools

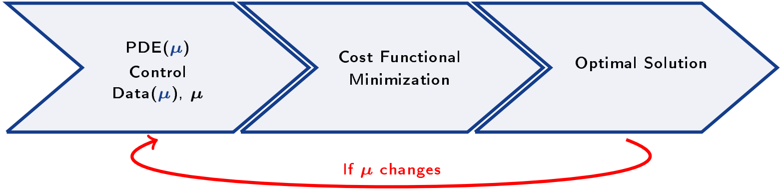
- *multiphenics (https://mathlab.sissa.it/multiphenics)*
- *RBniCS (https://www.rbnicsproject.org/)*

Motivations

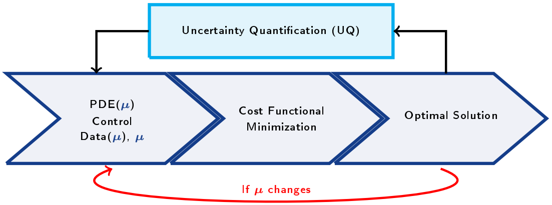
Reduced Order Model (ROM) for parameterized Optimal Flow Control Problems (OFCP($\boldsymbol{\mu}$))

- based on *data*
  (noisy, scattered, difficult to interpret...)
- several simulations for different values of physical and/or geometrical parameter $\boldsymbol{\mu}$
  (**uncertainty quantification**, **parameter estimation problems**...)

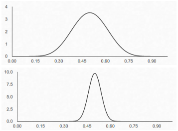
ROM: **fast** and **reliable** tool to solve several parametric instances;
OCP(μ): classical mathematical tool to **add data information** in the model.



ROMs for Uncertainty Quantification



- parameter is a random variable with given probability distribution ρ
- evaluation of some statistics on the optimal solution (expected solution) [Monte Carlo, a lot of realizations]
- using Weighted-ROM models to accelerate Monte Carlo methods
  - weight solutions during the construction of the ROM,
  - sample the parameter space during the construction of the ROM.



Problem Formulation

Continuous Problem Formulation

Problem: given $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^d$, find $(y(\boldsymbol{\mu}), u(\boldsymbol{\mu})) \in Y \times U$ which solves

$$\min_{(y,u)\in Y\times U} J(y,u;\boldsymbol{\mu}) := \min_{(y,u)\in Y\times U} \frac{1}{2}\|y(\boldsymbol{\mu}) - y_d(\boldsymbol{\mu})\|^2_{Y(\Omega_{\mathrm{OBS}})} + \frac{\alpha}{2}\|u(\boldsymbol{\mu})\|^2_{U(\Omega_u)}$$

$$\text{such that} \qquad L((y,u),w;\boldsymbol{\mu}) = \langle f(\boldsymbol{\mu}), w\rangle \; \forall w \in Y,$$

- Ω is our domain,
- Y, U are Hilbert Spaces,
- $\Omega_{\mathrm{OBS}} \subseteq \Omega$ is the *observation domain*,
- $\Omega_u \subseteq \bar{\Omega}$ is the *control domain*,
- $y_d(\boldsymbol{\mu}) \in Y(\Omega_{\mathrm{OBS}})$ is our given data in *observation space*,
- $\alpha > 0$ is a penalization parameter.

Continuous Problem Formulation

Problem: given $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^d$, find $(y(\boldsymbol{\mu}), u(\boldsymbol{\mu})) \in Y \times U$ which solves

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$$\text{such that} \qquad L((y, u), w; \boldsymbol{\mu}) = \langle f(\boldsymbol{\mu}), w \rangle \; \forall w \in Y,$$

Lagrangian Approach [p adjoint variable]

1) define $\mathcal{L}(y, u, p; \boldsymbol{\mu}) = J(y, u; \boldsymbol{\mu}) + L((y, u), p; \boldsymbol{\mu}) - \langle f(\boldsymbol{\mu}), p \rangle$

2) given $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^p$, find $(y, u, p) \in Y \times U \times Y$

$$\text{s.t.} \quad \begin{cases} \mathcal{D}_y \mathcal{L}(y, u, p; \boldsymbol{\mu})[z] = 0 & \forall z \in Y, \\ \mathcal{D}_u \mathcal{L}(y, u, p; \boldsymbol{\mu})[v] = 0 & \forall v \in U, \\ \mathcal{D}_p \mathcal{L}(y, u, p; \boldsymbol{\mu})[\kappa] = 0 & \forall \kappa \in Y. \end{cases}$$

Discretized Problem

Truth Problem: $\underbrace{\text{Spatial Discretization (FE) + Time Discretization (Euler)}}_{\mathcal{N}=N_h \cdot N_t}$

One-shot unsteady system

$$\begin{bmatrix} \mathsf{M}_y & 0 & \mathsf{B}^T \\ 0 & \alpha \mathsf{M}_u & -\mathsf{C}^T \\ \mathsf{B} & -\mathsf{C} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \Delta t \mathsf{M}_y \mathsf{y_d} \\ 0 \\ \Delta t \mathsf{f} \end{bmatrix}$$

$$\boldsymbol{y} = [y_1, \dots, y_{N_t}]$$
$$\boldsymbol{u} = [u_1, \dots, u_{N_t}]$$
$$\boldsymbol{p} = [p_1, \dots, p_{N_t}]$$

y, u, p FE discretization (dim $3\mathcal{N}$)

Discretized Problem

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$$\boldsymbol{p} = [p_1, \dots, p_{N_t}]$$

y, u, p FE discretization (dim $3\mathcal{N}$)

What is the real structure of the matrix?

Discretized Problem

Truth Problem: $\underbrace{\text{Spatial Discretization (FE) + Time Discretization (Euler)}}_{\mathcal{N}=N_h \cdot N_t}$

For example...(state equation)

$$
\mathsf{B} = \begin{bmatrix} \mathsf{M} + \Delta t \mathsf{D}(\boldsymbol{\mu}) & & & & \\ -\mathsf{M} & \mathsf{M} + \Delta t \mathsf{D}(\boldsymbol{\mu}) & & & \\ & -\mathsf{M} & \mathsf{M} + \Delta t \mathsf{D}(\boldsymbol{\mu}) & & \\ & & \ddots & \ddots & \\ & & & -\mathsf{M} & \mathsf{M} + \Delta t \mathsf{D}(\boldsymbol{\mu}) \end{bmatrix}
$$

$$
\mathsf{C} = \begin{bmatrix} \mathsf{C}_u(\boldsymbol{\mu}) & & & \\ & \mathsf{C}_u(\boldsymbol{\mu}) & & \\ & & \ddots & \\ & & & \mathsf{C}_u(\boldsymbol{\mu}) \end{bmatrix}
$$

Reduction could be very effective: **space-time** formulation is **unfeasible** for *real-time* applications.

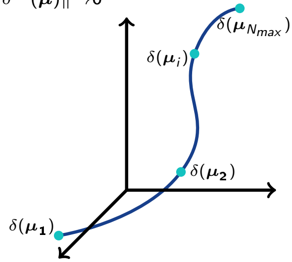
Methodology

Reduced Order Modelling for OCP(μ)s

Goal: to achieve the **accuracy** of the *truth* solution $\delta^{\mathcal{N}} = y^{\mathcal{N}}, u^{\mathcal{N}}, p^{\mathcal{N}}$ but at greatly **reduced cost** of a **low order model**.

Strategy: $\delta(\boldsymbol{\mu}) \xrightarrow{\text{Space-Time(dim}=\mathcal{N})} \delta^{\mathcal{N}}(\boldsymbol{\mu}) \xrightarrow[\|\delta(\boldsymbol{\mu})-\delta^{\mathcal{N}}(\boldsymbol{\mu})\|\to 0]{\text{ROM (dim } N)} \delta_N(\boldsymbol{\mu})$.

- Proper Orthogonal Decomposition (POD):
  - choose $N_{max} \subset \mathcal{D}$ finite,
  - pick $\delta^{\mathcal{N}}(\boldsymbol{\mu}^1), \dots, \delta^{\mathcal{N}}(\boldsymbol{\mu}^{N_{max}})$,
  - solve an eigenvalue problem on $\mathbb{C}_{ij} = \frac{1}{N_{max}}(\delta^{\mathcal{N}}(\boldsymbol{\mu}^i)\delta^{\mathcal{N}}(\boldsymbol{\mu}^j))$ for $i,j = 1, \dots, N_{max}$,
  - basis = eigenvectors associated to the largest N eigenvalues (aggragated spaces).



Important: $N \ll \mathcal{N}$

Weighted Reduced Strategies

Standard POD algorithm results in the optimal N-dimensional subspace of the variable space which minimizes

$$\int_{\mathcal{D}} \|\delta(\boldsymbol{\mu}) - \delta_N(\boldsymbol{\mu})\|^2 d\boldsymbol{\mu} \approx \frac{1}{N_{max}} \sum_{i=1}^{N_{max}} \|\delta(\boldsymbol{\mu}^i) - \delta_N(\boldsymbol{\mu}^i)\|^2,$$

Idea: use a more general quadrature rules of the form $\mathcal{U}(f) = \sum_{i=1}^{M} \omega^i f(\boldsymbol{\mu}^i)$ for every integrable function $f : \mathcal{D} \to \mathbb{R}$, where $\boldsymbol{\mu}^1, \dots, \boldsymbol{\mu}^N_{max} \in \mathcal{D}$ are the nodes of the quadrature and $\omega^1, \dots, \omega^N_{max}$are the respective weights.
This results in the following approximation:

$$\mathbb{E}\left[\|\delta - \delta_N\|^2\right] \approx \frac{1}{N_{max}} \sum_{i=1}^{N_{max}} \underbrace{\omega_i \rho(\boldsymbol{\mu}^i)}_{w(\mu^i)} \|\delta(\boldsymbol{\mu}^i) - \delta_N(\boldsymbol{\mu}^i)\|^2$$

How does it work? $\mathbb{C}_{ij} = \frac{1}{N_{max}}(\delta^{\mathcal{N}}(\boldsymbol{\mu}^i), \delta^{\mathcal{N}}(\boldsymbol{\mu}^j)) \to \mathbb{C}^w_{ij} = \frac{w(\boldsymbol{\mu}^i)}{N_{max}}(\delta^{\mathcal{N}}(\boldsymbol{\mu}^i), \delta^{\mathcal{N}}(\boldsymbol{\mu}^j))$

Some Examples of Nodes

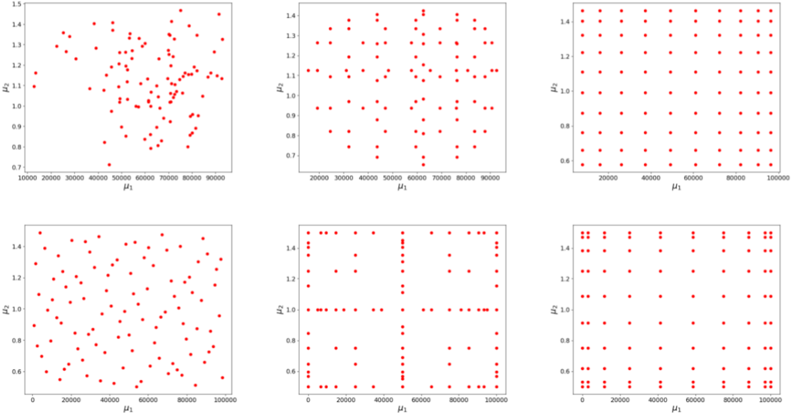


Figure: Nodes for different quadrature rules

Some Examples of Distributions

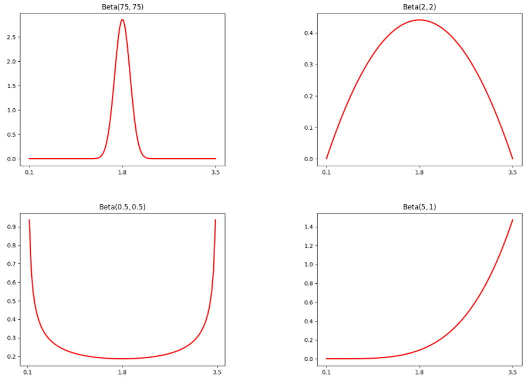


Figure: Different distributions

Applications and Numerical Results

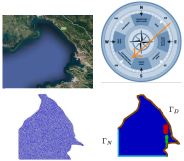
Pollutant Control on the Gulf of Trieste

Motivations: *monitor*, *manage* and predict dangerous marine phenomena in a *fast way*
Aim: pollutant loss $y \in H^1_{\Gamma_D}(\Omega)$ under a safeguard threshold y_d

Given $\boldsymbol{\mu} \in [0.5, 1] \times [-1, 1] \times [-1, 1]$, find $(y(\boldsymbol{\mu}), u(\boldsymbol{\mu})) \in Y \times U$ which solves

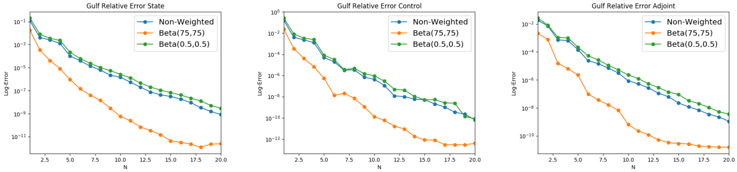
$$\min_{(y,u)} \frac{1}{2} \int_{\Omega_{OBS}} (y - y_d)^2 \, d\Omega_y + \frac{\alpha}{2} \int_{\Omega_u} u^2 \, d\Omega_u$$

$$\text{s.t.} \begin{cases} \mu_1 \Delta y + [\mu_2, \mu_3] \cdot \nabla y \, d\Omega = u \chi_{\Omega_u} & \text{in } \Omega \\ \frac{\partial y}{\partial n} = 0 & \text{on } \Gamma_N \\ y = 0 & \text{on } \Gamma_D \end{cases}$$



Boundaries:
Γ_D = coasts, Γ_N = Adriatic Sea.
Subdomains:
Ω_{OBS} = Natural area of Miramare;
Ω_u = Source of pollutant (in front of the city of Trieste).
$\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\mu}_3$: wind action, α: 10^{-5}, y_d: 0.2

Numerical Results



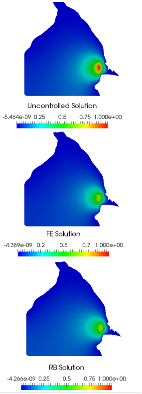


Figure: Relative Error for the state (left), control (middle), adjoint (right), using ordinary POD (blue), Beta(0.5, 0.5)-Weighted-POD (green), Beta(75, 75)-Weighted-POD (orange). Three different quadrature rules for Beta(75, 75).

[Carere, Strazzullo, Ballarin, Rozza, Stevenson. Weighted POD-reduction for parametrized PDE-constrained Optimal Control Problems with random inputs and its applications to environmental sciences, Computers & Mathematics with Applications, 2021.]

Stabilized State Equation

We deal with **Advection-Diffusion Problem** (High Péclet→ Stabilization (SUPG)):

$$L(\boldsymbol{\mu})y := y_t - \varepsilon(\boldsymbol{\mu})\Delta y + \mathrm{b}(\boldsymbol{\mu}) \cdot \nabla y \quad + \text{boundary conditions.}$$

Questions

Is OCP($\boldsymbol{\mu}$) able to avoid instabilities? (Do I still need stabilization? For the adjoint too?)
Is consistent FOM-ROM model convenient?
How can I introduce stochastic knowledge in model order reduction?

[Zoccolan, Strazzullo, Rozza, "A Streamline upwind Petrov-Galerkin Reduced Order Method for Advection-Dominated Partial Differential Equations under Optimal Control", submitted, 2023.]
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The SUPG stabilization for the whole system

[Collis, Heinkenschloss, Analysis of the Streamline Upwind/Petrov Galerkin method applied to the solution of optimal control problems. CAAM TR02-01, 108, 2002.]

Controlled state equation

$$a\left(y^{\mathcal{N}}, q^{\mathcal{N}}; \boldsymbol{\mu}\right) + \sum_{K \in \mathcal{T}_h} \delta_K \left(L y^{\mathcal{N}}, \frac{h_K}{|\mathrm{b}|} L_{SS} q^{\mathcal{N}}\right)_K - \int_\Omega u^{\mathcal{N}} q^{\mathcal{N}} - \sum_{K \in \mathcal{T}_h} \delta_K \left(u^{\mathcal{N}}, \frac{h_K}{|\mathrm{b}|} L_{SS} q^{\mathcal{N}}\right)_K$$
$$= \mathrm{f}(q^{\mathcal{N}}; \boldsymbol{\mu}) + \sum_{K \in \mathcal{T}_h} \delta_K \left(f, \tfrac{h_K}{|\mathrm{b}|} L_{SS} q^{\mathcal{N}}\right)_K \quad \forall q^{\mathcal{N}} \in Y^{\mathcal{N}}.$$

Gradient equation (not affected)

$$\alpha \int_\Omega u^{\mathcal{N}} v^{\mathcal{N}} \, \mathrm{dx} = \int_\Omega p^{\mathcal{N}} v^{\mathcal{N}} \, \mathrm{dx} \quad \forall v^{\mathcal{N}} \in U^{\mathcal{N}}$$

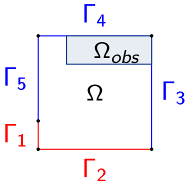
Adjoint equation

$$a^*\left(z^{\mathcal{N}}, p^{\mathcal{N}}\right) + \sum_{K \in \mathcal{T}_h} \delta_K \left(L^* p^{\mathcal{N}}, \frac{h_K}{|\mathrm{b}|} \left(-L_{SS}\right) z^{\mathcal{N}}\right)_K$$
$$+ \int_{\Omega_{obs}} (y^{\mathcal{N}} - y_d) z^{\mathcal{N}} \, \mathrm{dx} + \sum_{K \in \mathcal{T}_{h|\Omega_{obs}}} \delta_K \left(y^{\mathcal{N}} - y_d, \frac{h_K}{|\mathrm{b}|} \left(-L_{SS}\right) z^{\mathcal{N}}\right)_K = 0 \quad \forall z^{\mathcal{N}} \in Y^{\mathcal{N}}$$

Numerical Results

Given $\boldsymbol{\mu} \in \mathcal{P}$ find $\displaystyle \min_{(y,u)\in H^{(}0,T;H^1(\Omega))\times L^2(0,T:L^2(\Omega))} \frac{1}{2}\|y - y_d\|^2_{L^2(0,T;L^2(\Omega_{obs}))} + \frac{\alpha}{2}\|u\|^2_U$ such that

$$
\begin{cases}
y(\boldsymbol{\mu})_t - \dfrac{1}{\mu_1}\Delta y(\boldsymbol{\mu}) + (\cos \mu_2, \sin \mu_2)\cdot \nabla y(\boldsymbol{\mu}) = u, & \text{in } \Omega \times (0,T),\\
y(\boldsymbol{\mu}) = 1 & \text{on } \Gamma_1 \cup \Gamma_2 \times (0,T),\\
y(\boldsymbol{\mu}) = 0 & \text{on } \Gamma_3 \cup \Gamma_4 \cup \Gamma_5 \times (0,T),\\
y(\boldsymbol{\mu})(0) = 0 & \text{in } \Omega.
\end{cases}
$$



Data

$\Omega = (0,1)^2$, $T = 3$, $\Delta t = 0.1$, $N_t = 30$, $\mathcal{N} = 362610$, $y_d = 0.5$, $h = 0.036$, $\delta_k = 1.$, $\mathcal{P} = [10^2, 10^5] \times [0, 1.57]$, $\alpha = 0.01$, $N_{max} = 100$, $N = 30$.

Numerical Results (Deterministic)

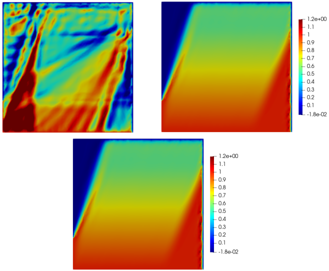


Figure: Only-Offline stabilized, Online-Offline vs FEM (bottom), $\mu = (2 \cdot 10^2, 1.2)$ at the final time.

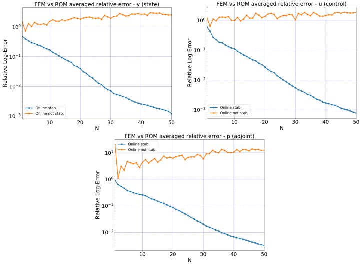
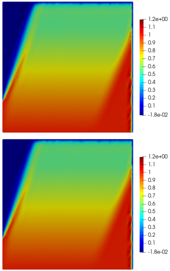


Figure: Relative errors between FEM and reduced solutions

Performances (FOM-ROM Stabilization is preferable)

Relative errors over time and parameters ($P_{train} = 100$) $\sim 10^{-2}, 10^{-3}$. Speedup ~ 5000

Numerical Results (Random Inputs)



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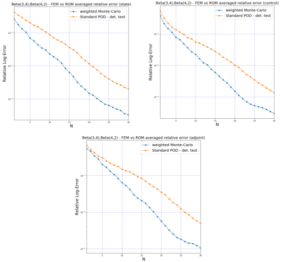
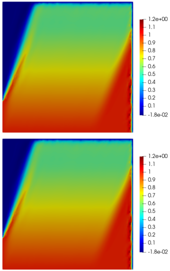


Figure: Relative errors between FEM and reduced solutions POD and w-POD (Beta(3,4), Beta(4,2))

At first we tried a steady case with different quadrature rules, but it was always better to sample as the distribution

Numerical Results (Random Inputs)



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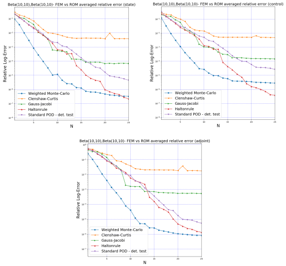


Figure: (Steady case) Relative errors between FEM and reduced solutions w-POD (Beta(10,10), Beta(10,10) and different quadrature points)

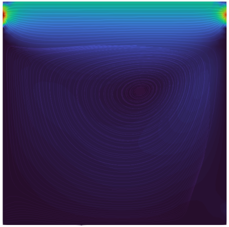
Performances (no sparse grids for time dependent)

The error value 10^{-3} is reached for $N = 30$ (and not 50).

Future Directions

Multi-fidelity Statistical POD for OCP

Goal: accelerate the offline phase



- Dirichlet control
- Part of the snapshots collected by optimal control problems
- Part of the snapshots collected by uncontrolled system with random Dirichlet inputs

Results: fast construction + not loosing accuracy
Collaborator: Enrique Delgado (University of Seville)

[Dolgov, Kalise, Saluzzi, "Statistical Proper Orthogonal Decomposition for model reduction in feedback control", arxiv preprint, 2023.]

Dynamical Orthogonal Reduced Basis for Feedback Control

Given a set of initial conditions find the state solution $\mathcal{Y} \in \mathcal{C}^1((0,\infty), \mathbb{R}^{N_h \times p})$ such that

$$\begin{cases} \delta\mathcal{Y}(t) = A\mathcal{Y}(t) + Bu(\mathcal{Y}(t)) & \text{for } t \in (0,\infty) \\ \mathcal{Y}(t_0) = \mathcal{Y}_0(\mu). \end{cases} \tag{1}$$

The main objective is to represent $\mathcal{Y}(t)$ in a **dynamical reduced space**

$$\mathcal{Y}(t) \approx \mathsf{Y}(t) = \mathsf{U}(t)\mathsf{Z}^T(t) = \sum_{i=1}^{n} U_i(t) Z_i(t;\mu), \tag{2}$$

Results: more accurate results and more comprehensive view of the optimality system
Collaborators: Cecilia Pagliantini (University of Pisa) and Luca Saluzzi (Scuola Normale Superiore di Pisa)

[Sapsis, Lermusiaux, "Dynamically orthogonal field equations for continuous stochastic dynamical systems", Physica D, 2009.]

Conclusions and Perspectives

- Optimal Control in UQ,
- w-ROM,
- munerical results in environmental science and convection-dominated regime.

... More to be done

- Boundary Control,
- deeper analysis of the role of the control and different techniques,
- data-driven and non-intrusive techniques,

Acknowledgements

European Union Funding for Research and Innovation – Horizon 2020 Program – in the framework of European Research Council Executive Agency: Consolidator Grant H2020 ERC CoG 2015 AROMA-CFD project 681447 "Advanced Reduced Order Methods with Applications in Computational Fluid Dynamics".

Thank you for your attention

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