Data-driven reduced order methods in CFD enhanced by unsupervised parameters reduction

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Introduction

We present two computational pipelines able to enhance data-driven reduced order methods, exploiting the presence of active subspaces (AS). The first one, in column A, couples proper orthogonal decomposition with interpolation and AS for the reconstruction of the pressure modal coefficients. The second one, in column B, uses dynamic mode decomposition for future-state prediction of the lift coefficient, and dynamical AS to identify unnecessary parameters and build a more precise Gaussian Process Regression (GPR) in a lower dimensional space. Both pipelines are applied in CFD context using Finite Volume method, and automatic mesh morphing with free form deformation and radial basis functions interpolation.

1 - Active Subspace (AS) Property [1]

Consider a function, its gradient vector and a sampling density

$$f = f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^m, \quad \nabla f(\mathbf{x}) \in \mathbb{R}^m, \quad \rho : \mathbb{R}^m \to \mathbb{R}_+$$

Take the average outer product of the gradients and partition its decomposition,

$$\mathbf{C} = \mathbb{E}\left[\nabla_{\mathbf{x}} f \, \nabla_{\mathbf{x}} f^T\right] = \int (\nabla_{\mathbf{x}} f)(\nabla_{\mathbf{x}} f)^T \rho \, d\mathbf{x} = \mathbf{W} \mathbf{\Lambda} \mathbf{W}^T$$

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & \\ & \mathbf{\Lambda}_2 \end{bmatrix}, \qquad \mathbf{W} = [\mathbf{W}_1 \quad \mathbf{W}_2], \qquad \mathbf{W}_1 \in \mathbb{R}^{m \times n}$$

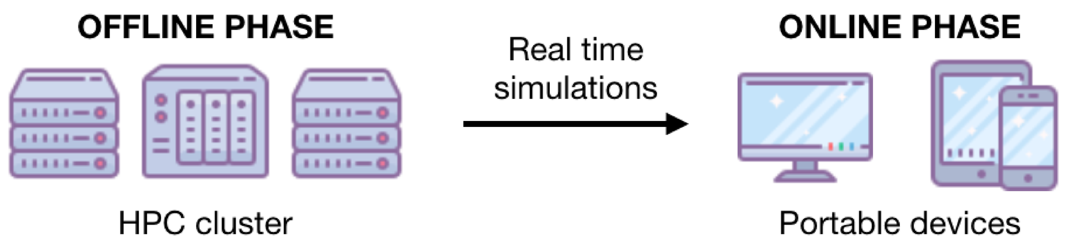
Rotate and separate the coordinates: $\mathbf{x} = \mathbf{W}\mathbf{W}^T\mathbf{x} = \mathbf{W}_1\mathbf{W}_1^T\mathbf{x} + \mathbf{W}_2\mathbf{W}_2^T\mathbf{x} = \mathbf{W}_1\mathbf{y} + \mathbf{W}_2\mathbf{z}$.
We have that $\mathbf{y}$ is the active variable and $\mathbf{z}$ the inactive one:

$$\mathbf{y} = \mathbf{W}_1^T\mathbf{x} \in \mathbb{R}^n, \qquad \mathbf{z} = \mathbf{W}_2^T\mathbf{x} \in \mathbb{R}^{m-n}$$

2A - POD with interpolation (PODI)

POD with interpolation main features:

- No need to know the underlying equations/matrices (as for POD-Galerkin method)
- SVD of the snapshots matrix $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^*$
- Using the first N modes, we are able to span the low-dimensional space on which we project the original samples. The **modal coefficients** are: $\mathbf{C} = \mathbf{U}_N^T\mathbf{X}$
- Real-time computation of the solution fields for any new parameter by interpolating the modal coefficients
- **Offline-online paradigm** allows to efficiently exploit all the collected simulations (moreover we can enrich the database!)

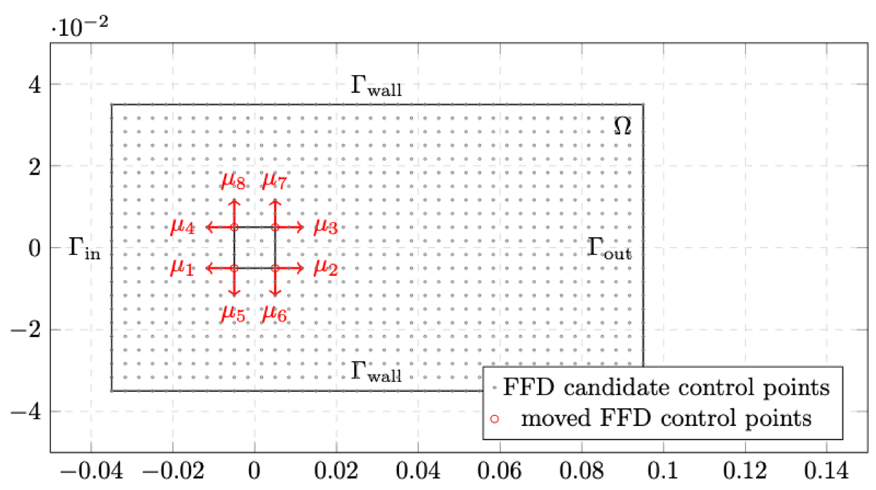


2B - Dynamic mode decomposition (DMD)

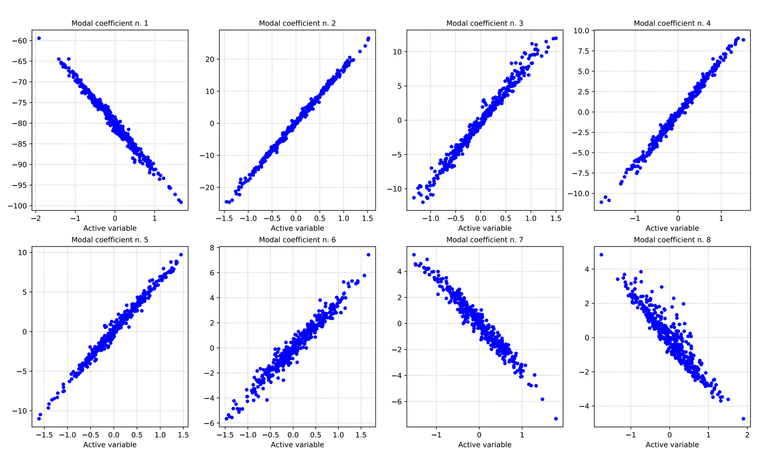
1. **Collection of the snapshots**
   - Creation of two matrices: snapshots ($\mathbf{X}$) and time-shifted snapshots ($\mathbf{Y}$)
2. **Eigenvalues and modes computation**
   - Approximation of the operator $\mathbf{A}$ — $\mathbf{Y} \approx \mathbf{A}\mathbf{X}$
   - SVD of the snapshots matrix — $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^*$
   - Reduction of the operator — $\tilde{\mathbf{A}} = \mathbf{U}^*\mathbf{Y}\mathbf{V}\mathbf{\Sigma}^{-1}$
   - Eigendecomposition — $\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\mathbf{\Lambda}$
   - Computation of the modes — $\mathbf{\Phi} = \mathbf{Y}\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{W}$, $\mathbf{\Phi} = \mathbf{U}\mathbf{W}$
3. **Reconstruction and prediction**
   - Computation of the amplitudes $\mathbf{b}$
   - Midcasting and forecasting — $\mathbf{x}_k = \mathbf{\Phi}\mathbf{\Lambda}^k\mathbf{b}$

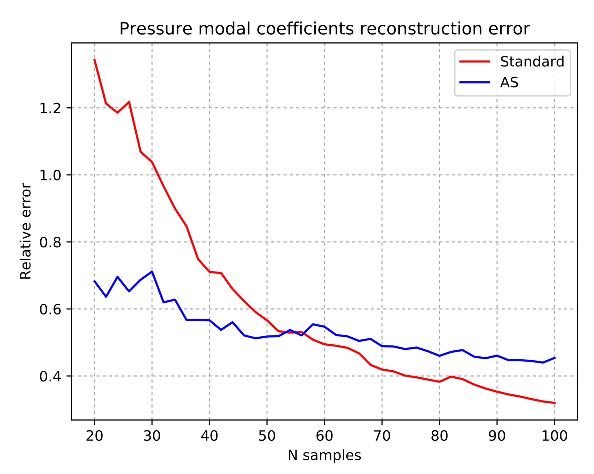
3A - Modal coefficient approximation with AS [2]

We reconstruct the pressure field for a parametrized domain with free form deformation using PODI.



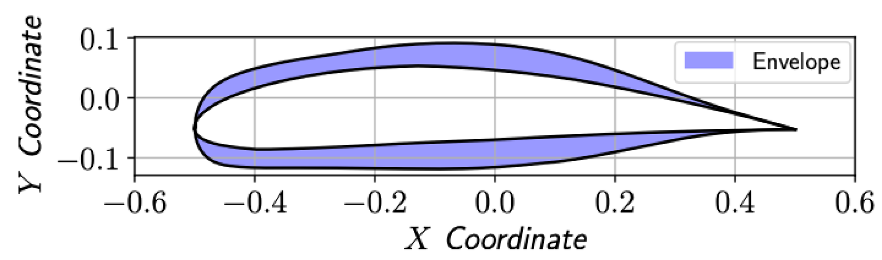
We exploit AS for the approximation of the first 8 modal coefficient. This results in a more accurate field reconstruction for small computational budget up to 55 samples in the 8-dimensional parameter space.

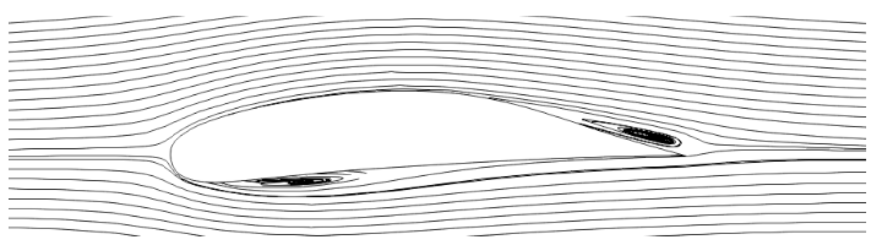




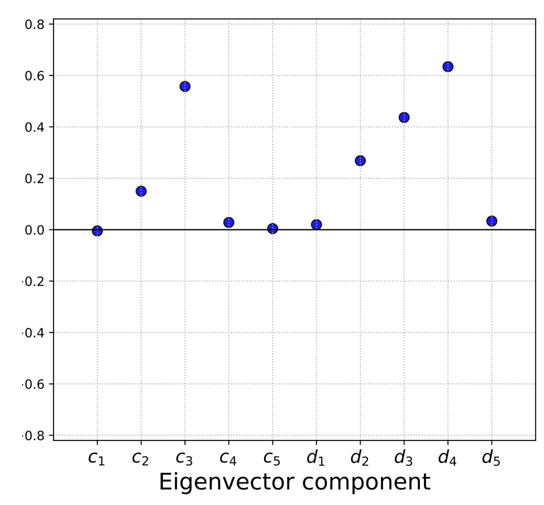
3B - GP regression for DMD enhanced by AS [3]

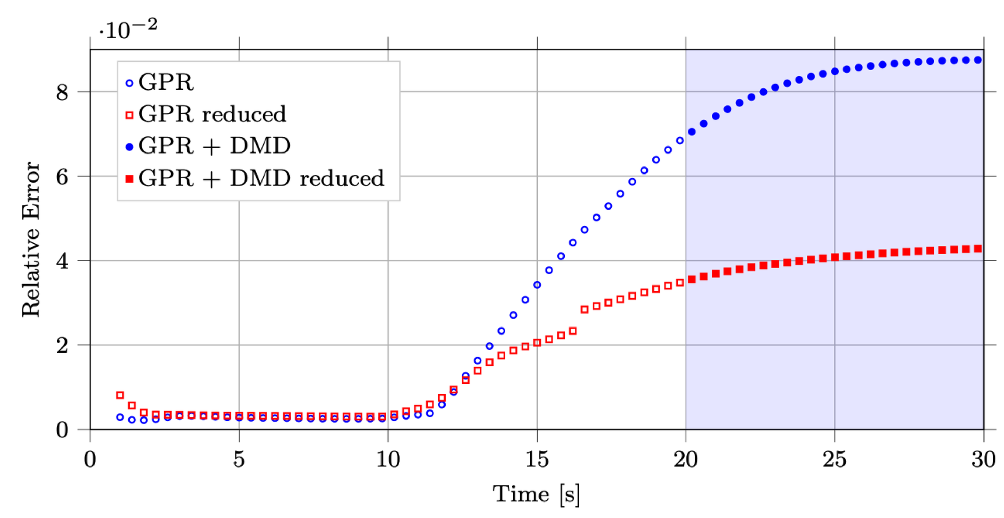
We parametrize a NACA 4412 airfoil profile and automatically deform the computational mesh with RBF interpolation. Here the envelope of the deformations and the flow velocity streamlines.





We study the evolution in time of the AS coefficients for the lift and identify 4 parameters with little to no influence on average. By freezing these parameters we improve the GPR capabilities even for future-state prediction with DMD.
DMD and AS training done with the first 20 s of the time-varying lift coefficient for 70 different morphed airfoils.





4 - Computational science and engineering softwares: `mathlab.sissa.it/cse-software`

PyGeM
github.com/mathLab/PyGeM
mathlab.github.io/PyGeM

PyGeM is a python package using Free Form Deformation, Radial Basis Functions, and Inverse Distance Weighting to morph complex geometries.

PyDMD
github.com/mathLab/PyDMD
mathlab.github.io/PyDMD

PyDMD is a Python package that uses Dynamic Mode Decomposition for a data-driven model simplification based on spatiotemporal coherent structures.

ITHACA-FV
github.com/mathLab/ITHACA-FV
mathlab.github.io/ITHACA-FV

ITHACA-FV is an implementation in OpenFOAM of several reduced order modeling techniques based on Finite Volume method.

EZyRB
github.com/mathLab/EZyRB
mathlab.github.io/EZyRB

EZyRB is a python library for data-driven (non-intrusive) model order reduction with POD with interpolation.

References and Acknowledgements

[1] P. G. Constantine. *Active subspaces: Emerging ideas for dimension reduction in parameter studies*, volume 2 of *SIAM Spotlights*. SIAM, 2015.

[2] N. Demo, M. Tezzele, and G. Rozza. A non-intrusive approach for proper orthogonal decomposition modal coefficients reconstruction through active subspaces. *Comptes Rendus de l'Académie des Sciences DataBEST 2019 Special Issue*, 2019.

[3] M. Tezzele, N. Demo, G. Stabile, A. Mola, and G. Rozza. Enhancing CFD predictions in shape design problems by model and parameter space reduction. *Advanced Modeling and Simulation in Engineering Sciences*, 2019.

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