Parameter space and model reduction with shape parametrization, by means of active subspaces and POD-Galerkin methods for industrial and biomedical applications

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Introduction

We introduce a new framework for parameters space reduction in naval and biomedical engineering obtained by coupling: Active Subspaces property to identify lower dimensional structure in the parameters space [1]; Free Form Deformation (FFD) and Radial Basis Functions (RBF), to morph the geometry; Response surfaces method (RS) and POD-Galerkin methods.

The Active Subspaces Property

Consider a function, its gradient vector and a sampling density

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

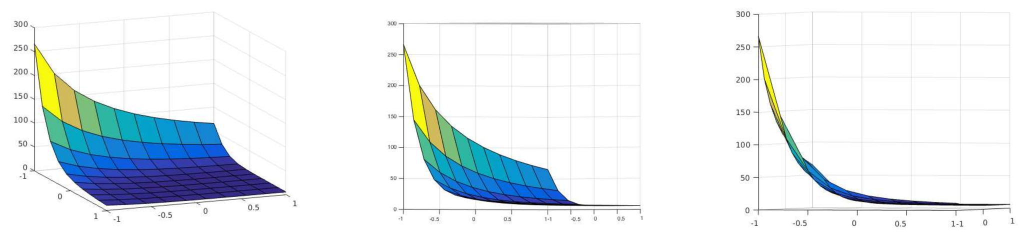
Take the average outer product of the gradient and partition its eigendecomposition,

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

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

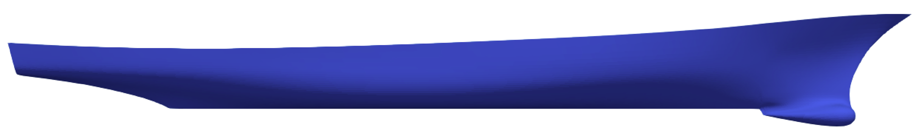
Rotate and separate the coordinates: $\mathbf{x} = \mathbf{W}\mathbf{W}^T\mathbf{x} = \mathbf{W}_1\mathbf{W}_1^T\mathbf{x} + \mathbf{W}_2\mathbf{W}_2^T\mathbf{x} = \mathbf{W}_1\mathbf{y} + \mathbf{W}_2\mathbf{z}$.

We have that $\mathbf{y} = \mathbf{W}_1^T\mathbf{x} \in \mathbb{R}^n$ is the active variable and $\mathbf{z} = \mathbf{W}_2^T\mathbf{x} \in \mathbb{R}^{m-n}$ the inactive one.



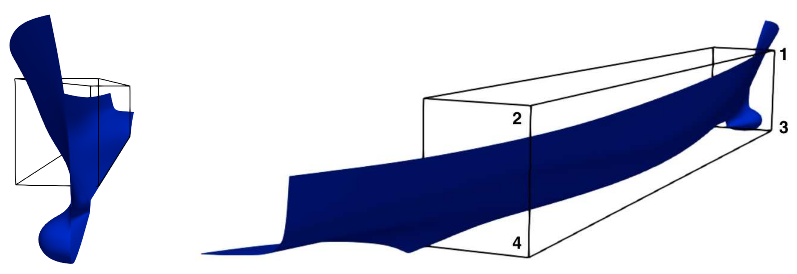
A parametric version of the DTMB 5415 hull

The DTMB 5415 is a hull conceived for preliminary design of a US Navy Combatant and it is a very common benchmark for the validation of CFD models. The hull geometry includes both a sonar dome and transom stern.



As geometrical parameters we select 6 components of 4 control points of a FFD lattice over one side wall of the hull and we apply the same deformation to the other side. The structural parameter is the displacement of the hull and the physical one is the velocity.

Parameter	Nature	Lower bound	Upper bound
u_1	FFD Point 1 y	-0.2	0.3
u_2	FFD Point 2 y	-0.2	0.3
u_3	FFD Point 3 y	-0.2	0.3
u_4	FFD Point 4 y	-0.2	0.3
u_5	FFD Point 3 z	-0.2	0.5
u_6	FFD Point 4 z	-0.2	0.5
u_7	weight (kg)	500	800
u_8	velocity (m/s)	1.87	2.70

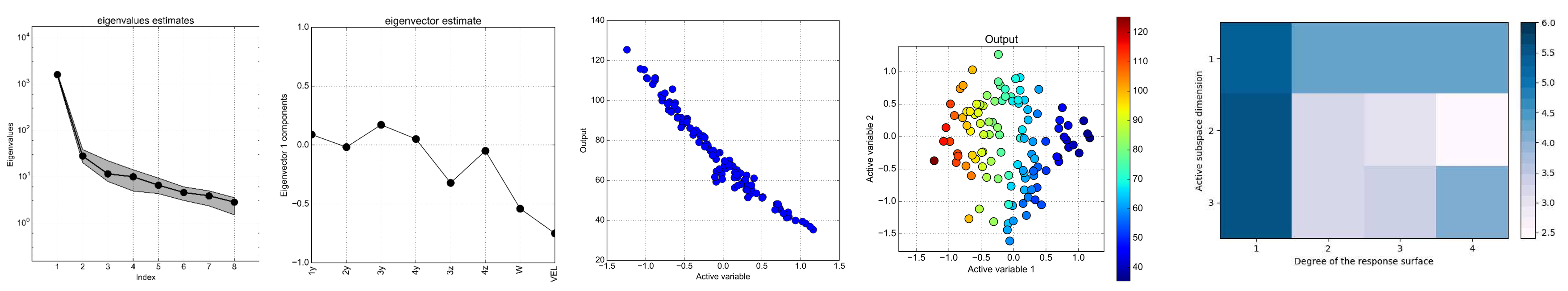


Eigenvalues and error analysis

We approximate the gradients of the wave resistance with respect to the parameters and look for a spectral gap of the $\mathbf{C}$ matrix.

We underline the presence of a major gap between the first and the second eigenvalue and a minor one between the second and the third.

The sufficient summary plot ($f(\mathbf{x})$ against $\mathbf{W}_1^T\mathbf{x}$) confirms the presence of an active subspace of dimension 1 and 2.



Using a response surface of order 4 and an active subspace of dimension 2 ensures an error on the test dataset equal to 2.5%. It is a good starting point to perform further optimization in the ridge approximation context. Doing so we reduced the parameter space from dimension 8 to 2.

Geometrical Deformation: the PyGeM library

PyGeM is a python library using Free Form Deformation, Inverse Distance Weighting, and Radial Basis Function interpolation to parametrize and morph complex geometries.

It interacts with industrial file formats used for CAD management (.iges, .step, .stl), mesh files (.unv and OpenFOAM), and output files (.vtk). See `github.com/mathLab/PyGeM` and `mathlab.sissa.it/cse-software`

Carotid parametrization

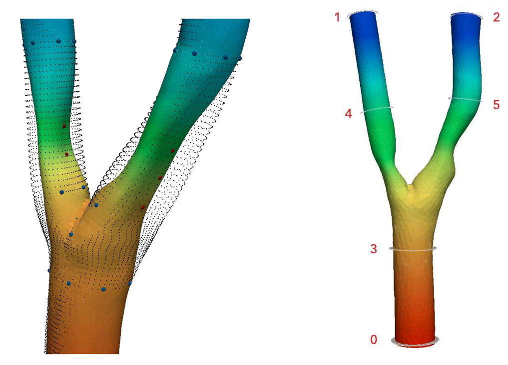
Vessels geometry strongly influences hemodynamics behaviour. We study the influence of the vessel shape on blood flow.

$$\begin{cases} -\nu \Delta \boldsymbol{u}(\boldsymbol{\mu}) + \boldsymbol{u}(\boldsymbol{\mu}) \cdot \nabla \boldsymbol{u}(\boldsymbol{\mu}) + \nabla p(\boldsymbol{\mu}) = \mathbf{0} & \text{in } \Omega(\boldsymbol{\mu}), \\ \text{div } \boldsymbol{u}(\boldsymbol{\mu}) = 0 & \text{in } \Omega(\boldsymbol{\mu}), \\ \boldsymbol{u}(\boldsymbol{\mu}) = \boldsymbol{u}_{\text{in}} & \text{on } \Gamma_{\text{in}}, \\ \boldsymbol{u}(\boldsymbol{\mu}) = \mathbf{0}, & \text{on } \Gamma_{\text{wall}}(\boldsymbol{\mu}), \\ \nu \dfrac{\partial \boldsymbol{u}(\boldsymbol{\mu})}{\partial \boldsymbol{n}} - p(\boldsymbol{\mu})\boldsymbol{n} = \mathbf{0}, & \text{on } \Gamma_{\text{out}}, \end{cases}$$

In particular we want to simulate an occlusion.

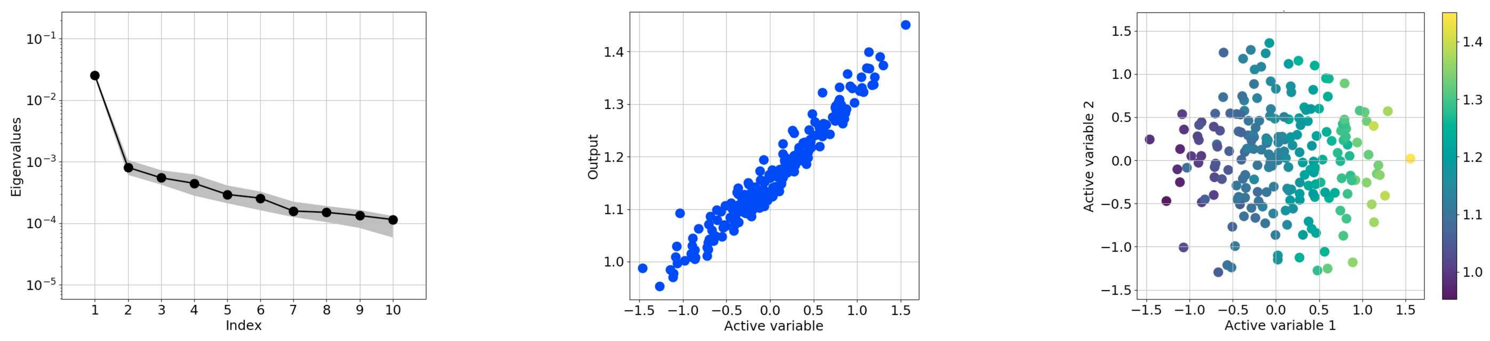
We deform the carotid after the bifurcation moving 10 RBF control points (in red) solving an interpolation system.

The output function is the relative pressure drop of the two branches, computing the integral of the pressure on the highlighted sections.



Spectral and POD analysis

The presence of an active subspace of dimension one is clear both from the spectral analysis and the sufficient summary plot.

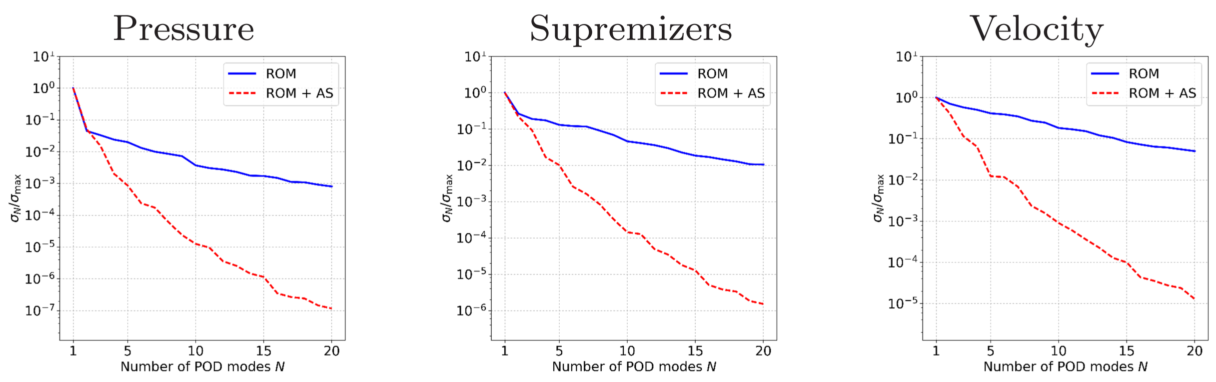


The two dimensional active subspace spanned by the first two eigenvectors of the covariance matrix seems to better capture the behaviour of the output function. We use this information perform a further reduction by a POD-Galerkin ROM.

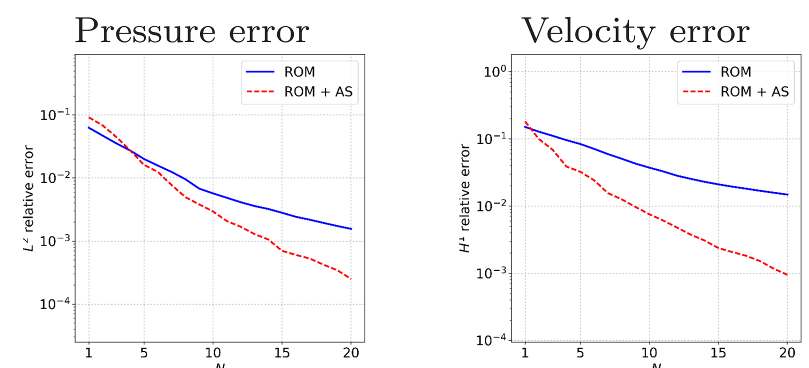
We exploit a 2-dimensional active subspace to compute the POD snapshots in a reduced space with respect to the full 10-dimensional parameter space.

Typical reduced space dimensions and computational speedup for cardiovascular flows. In particular the speedup from high-fidelity simulations to reduced-order ones: 500:1.

Here the POD singular values for velocity, supremizers and pressure, as a function of the number N of selected POD modes:



The results show a slower decay for the standard approach when compared to the combined one, meaning that the standard approach has to deal with a considerably larger solution manifold.



The combined methodology is able to reach relative errors which are up to an order of magnitude smaller when compared to the standard one, for both velocity and pressure when $N = 20$.

References

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

[2] M. Tezzele, F. Ballarin, and G. Rozza. Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD-Galerkin methods. *Submitted; preprint arXiv:1711.10884*, 2017.

[3] M. Tezzele, N. Demo, M. Gadalla, A. Mola, and G. Rozza. Model order reduction by means of active subspaces and dynamic mode decomposition for parametric hull shape design hydrodynamics. *Submitted; preprint arXiv:1803.07377*, 2018.

[4] M. Tezzele, F. Salmoiraghi, A. Mola, and G. Rozza. Dimension reduction in heterogeneous parametric spaces with application to naval engineering shape design problems. *Submitted; preprint arXiv:1709.03298*, 2017.

Acknowledgements

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