Scientific Computing Enhanced by Model Order Reduction and Machine Learning:

state of the art, perspectives, challenges and applications:

Gianluigi Rozza
grozza@sissa.it

MathLab, Mathematics Area, SISSA International School for Advanced Studies, Trieste, Italy

RTTE CNRS
Courcimont, France

6 November 2024

Motivations

#problems #state-of-the-art #applications #needs

Acknowledgements for the presentation setting:
Moaad Khamlich, Anna Ivagnes, Pierfrancesco Siena, Marco Tezzele, Caterina Balzotti, Michele Girfoglio, Federico Pichi, Maria Strazzullo

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Leading Motivation: computational science and engineering challenges

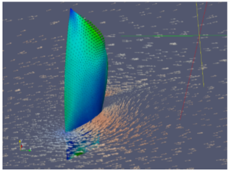
Numerical simulations are a booming field for mathematics and computational modelling.

They are able to deal with **multiphysics** problems, as well as systems characterized by **multiple spatial and temporal scales**.

In fact, in the last years, by both **industrial and clinical** research partners there is a growing demand of:

* **efficient computational tools** for
* **many query** and **real time** computations,
* **parametrized formulations**,
* simulations of increasingly **complex systems** with uncertain scenarios

There is a clear need of a computational collaboration rather than a competition between **High Performance Computing** (HPC) and **Reduced Order Methods** (ROM), as well as Full/High Order and Reduced Order Methods!



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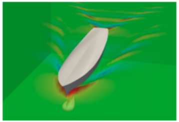
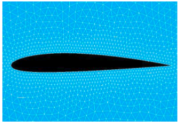
Overview of the physical parametric problems

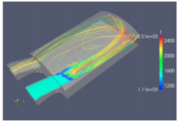
Industrial Flows



Naval Eng.

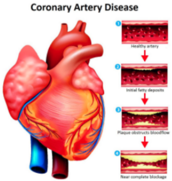


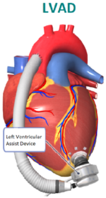
Aeronautics

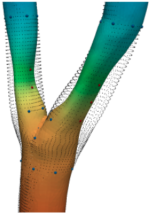


Industrial App.

Biomedical Applications







The fields of application are many: **naval**, **nautical, mechanical, civil**, **aeronautical**, **industrial** as well as **biomedical engineering**.

More in general, the response any application is going to deal with a wide range of parameters, both **dimensionless numbers** and **geometrical parameters**.

SISSA mathLab: our current efforts, aims and perspectives

A team developing **Advanced Reduced Order Methods** for parametric PDEs with a special focus on **Computational Fluid Dynamics**.

SISSA mathLab: our current efforts, aims and perspectives

Goals of our research group:

- to face and overcome **several limitations** of the **state of the art** for parametric ROM in CFD;
- to improve capabilities of reduced order methodologies for **more demanding applications** in **industrial**, **medical** and **applied sciences settings**;
- to carry out important methodological developments in **Numerical Analysis**, with special emphasis on mathematical modelling and a more extensive exploitation of **Computational Science and Engineering**
- focus on **Computational Fluid Dynamics** as a central topic to enhance broader applications in **multiphysics** and **coupled settings**, as well as more realistic models (e.g. aeronautical, mechanical, naval, off-shore, wind, sport, biomedical engineering and also cardiovascular surgery planning).



Applications of ROMs to Naval, Biomedical and Environmental fields

#ROM #Naval #Cardio #Environment

Gianluigi Rozza grozza@sissa.it

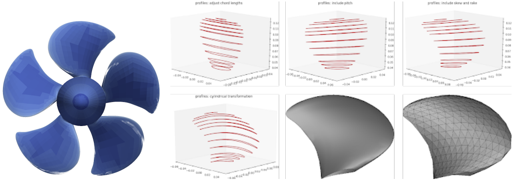
Motivations: Naval Projects

SOPHYA

Seakeeping Of Pleaning Hull YAchts

(in cooperation with MCY MONTECARLOYACHTS and MICAD MARINE INNOVATION CONSULTING AND DESIGN)

The main goal is to obtain a **hull of optimal shape** to improve the seakindness and comfort of the planing hulls in non calm sea conditions.



Python package developed: BladeX

prelica

Reduction of noise generated by propellers

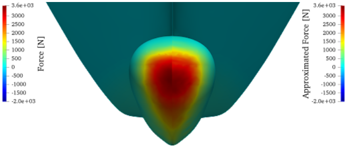
(in cooperation with FLUIDS and CETENA S.p.A.)

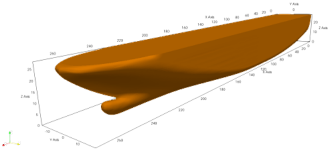
The aim of the project was to predict and reduce the **hydro-acoustic noise** generated by propeller blades and obtain a blade reliable parametrization and deformation.

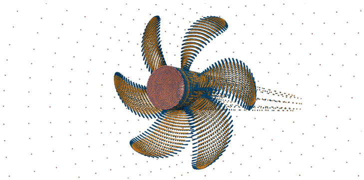
Data-driven Hull Shape Optimization System

(in cooperation with FINCANTIERI)

The aim was to develop an efficient shape optimization framework to reduce the hydrodinamic ship resistance. The aim is to achieve a remarkable reduction of the fuel consumption in the new cruise ships by optimized **hull shapes**.







Data-driven ROMs for blade shape optimization

(in cooperation with FINCANTIERI)

The aim of the project is to develop the shape that maximizes the **efficiency** of the propeller in cruise ships, avoiding the erosion and the cavitation phenomenon (formation of vapor-filled cavities).

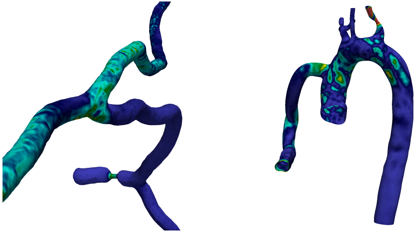
Python packages maintained: BladeX PyGeM

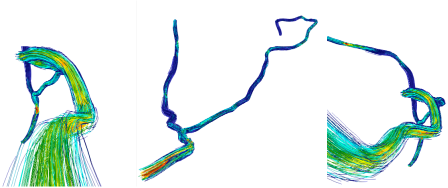
Motivations: Biomedical Projects

Data-driven ROMs for patient-specific data.

(in cooperation with Ospedale Luigi Sacco)

The aim was to develop an efficient ROM framework to reduce the computational time. The aim is to achieve a **real time evaluation** to choose the best **surgical plan**. **Speed-up**: $\mathcal{O}(10^5)$.





Data-driven ROMs for optimal control problem.

(in cooperation with University of HOUSTON)

The aim of the project is to develop a framework with the control on the **outlet boundary conditions**. **Speed-up**: $\mathcal{O}(10^4)$.

P. Siena, M. Girfoglio, F. Ballarin, G. Rozza, "Data-driven reduced order modelling for patient-specific hemodynamics of coronary artery bypass grafts with physical and geometrical parameters", J. Scie. Comp., 2023

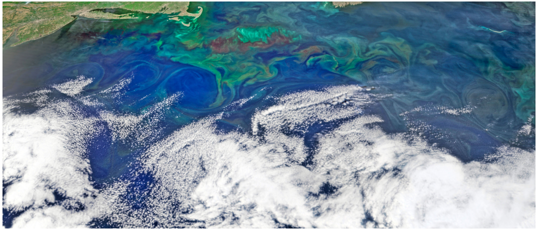
C. Balzotti, P. Siena, M. Girfoglio, A. Quaini, G. Rozza, "A data-driven Reduced Order Method for parametric optimal blood flow control: application to coronary bypass graft", COT Optimization, 2023

C. Balzotti, P. Siena, M. Girfoglio, G. Stabile, J. Dueñas-Pamplona, J. Sierra-Pallares, I. Amat-Santos, G. Rozza, "A Reduced Order model formulation for left atrium flow: an atrial fibrilaltion case", Sumbitted, 2023.

Motivations: Environmental Projects

ROMs for atmospheric and ocean flows
(in cooperation with University of HOUSTON)

The interest is in **geophysical flows** for **ocean** and **weather forecast**. We propose a framework which combines **ROM** and **LES**, and leads to a **Speed-up** ≈ 100 for **long time predictions**.
Recent work with Michele Girfoglio and Annalisa Quaini on JCP, 2023; JCAM, 2022.



Pollutant Control in the Gulf of Trieste

The goal is to monitor, manage and predict dangerous marine phenomena in a **fast way**. In particular we want to keep the pollutant loss under a safeguard **threshold**.
Works with Maria Strazzullo, Francesco Ballarin et al.

Overview

#technology #software #webcomputing
#offline-online #fast-computing

Gianluigi Rozza grozza@sissa.it

Intrusive Reduced Order Methods: a brief overview

- $()_h$: **Full Order Methods** (FEM, FV, FD, SEM) are **high fidelity solutions** - to be **accelerated**;
- $()^{ROM}$: **Reduced Order Methods** (ROM) - the **accelerator**.

- Input parameters:

$$\boldsymbol{\mu} \text{ (geometry, physical properties, etc.)}$$

- Parametrized PDE:

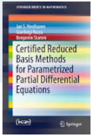
$$\mathcal{A}(u(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \rightsquigarrow \quad \underbrace{\boldsymbol{A}_h(\boldsymbol{\mu})\boldsymbol{u}_h(\boldsymbol{\mu}) = 0}_{\text{full order}} \quad \rightsquigarrow \quad \underbrace{\boldsymbol{A}^{ROM}(\boldsymbol{\mu})\boldsymbol{u}^{ROM}(\boldsymbol{\mu}) = 0}_{\text{reduced order}}$$

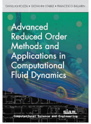
- Output:

$$u(\boldsymbol{\mu}) \quad \approx \quad \underbrace{\mathbf{u}_h(\boldsymbol{\mu})}_{\text{full order}} \quad \approx \quad \underbrace{\mathbf{u}^{ROM}(\boldsymbol{\mu})}_{\text{reduced order}}$$

- Input-Output evaluation:
  (black-box)

$$\boldsymbol{\mu} \quad \rightarrow \quad \mathbf{u}_h(\boldsymbol{\mu}) \quad \rightarrow \quad \mathbf{u}^{ROM}(\boldsymbol{\mu})$$





J. S. Hesthaven, G. Rozza, and B. Stamm., "Certified Reduced Basis Methods for Parametrized Partial Differential Equations", SpringerBriefs in Mathematics, Springer, 2015

P. Benner, W. Schilders, S. Grivet-Talocia, A. Quarteroni, G. Rozza, and L. M. Silveira , "Model Order Reduction, Volume 1,2,3", De Gruyter, 2020

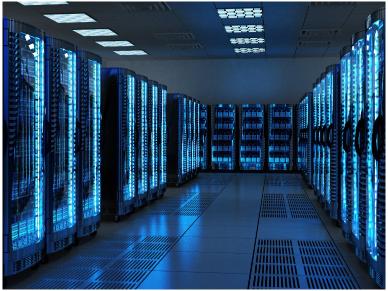
J. S. Hesthaven, C. Pagliantini, and G. Rozza, "Reduced basis methods for time-dependent problems", Acta Numerica, 2022

G. Rozza, G. Stabile, and F. Ballarin, "Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics", SIAM Press, 2022

ROMs: towards real-time computation (hardware)

Towards **Real-Time Computing** and Visualization, through an Offline–Online computational paradigm.

OFFLINE (full order)
High Performance Computing



* **Very expensive** and time demanding;
* basis calculation done once after suitable parameters sampling (ex: **Proper Orthogonal Decomposition, RB, PGD**, ...);
* *HPC facilities*.

ONLINE (reduced order)
Advanced ROM techniques

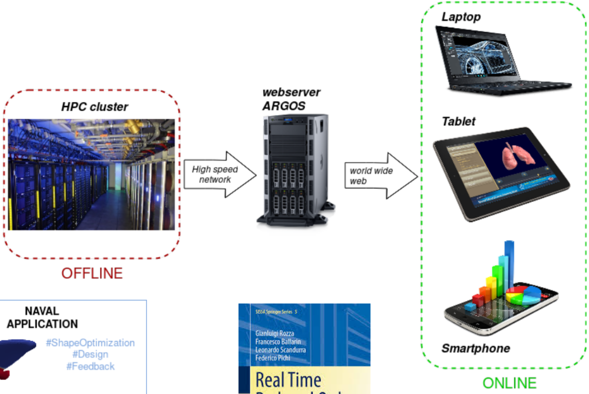
* **Extremely fast**;
* **real-time** input-output evaluation;
* computational **webserver** via browser;
* *in situ, tablets or smartphones*.

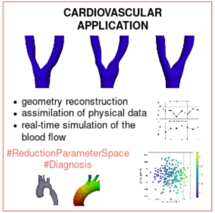
Gianluigi Rozza grozza@sissa.it

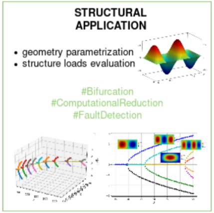
Future Perspectives: to real-time web computing (ARGOS ERC PoC)

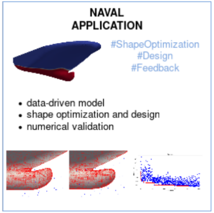
Model order reduction for computational web server: to real world applications argos-edu.sissa.it

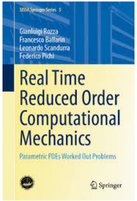
* HPC
* data science
* Digital twin
* SMACT Industry 4.0
* 3D Printing











FAST COMPUTING

ROMs: libraries developed at SISSA mathLab (software)

* Development of new high-quality **open source software libraries** [1], that can be freely employed and extended by anyone around the world, and are now the basis of teaching activities, collaborations and projects with several academic and industrial partners.
* High-level integration of newly developed reduced order methods with an already existing computational pipeline, in order to propose to use all the scientific developments carried out in the **ERC AROMA-CFD project** as an add-on onto the existing computational pipeline, rather than a completely different one.

[1] **mathlab.sissa.it/cse-software**

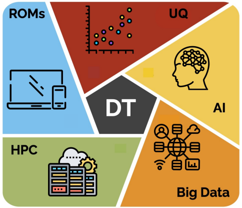
Digital Twin (DT): integration of emerging fields

A large amount of data (**Big Data**) can be collected, **Artificial Intelligence** (AI) can help to store and **organize** them (data-driven approaches).

By using **black box models**, AI techniques are able to find **fitting functions**. They do not require knowledge about the physics of the problem, even if we do prefer integrated "**Big Models**" Physics informed approaches.

The development of **High Performance Computing** (HPC) and its integration with reduced order models allowed to reach better performances.

* **Uncertainty quantification** (UQ),
* **Data analytics**,
* **Artificial intelligence** (AI),
* **Digital Twins** of products and processes.



Thanks to ROMs we have a more sustainable framework, energy savings, reduced computational times and resources.

Reduced basis (RB) vs Proper Orthogonal Decomposition (POD)

Full Order Model: $\boldsymbol{A}_h(\boldsymbol{\mu})\boldsymbol{u}_h(\boldsymbol{\mu}) = 0$ with $\mathbf{u}_h \in \mathbb{V}_h$ and $dim(\mathbb{V}_h) = N_h$
Parameters: $\boldsymbol{\mu}_i \in [\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_N]_{off}$
High-fidelity solutions: $\boldsymbol{u}_h^i = \boldsymbol{u}_h(\boldsymbol{\mu}_i)$

Proper Orthogonal Decomposition:

- **Eigenvalue problem**:

$$\boldsymbol{C}_{ij} = (\boldsymbol{u}_h^i)^T \boldsymbol{M} \boldsymbol{u}_h^j \quad \rightarrow \quad \boldsymbol{C}\boldsymbol{V} = \boldsymbol{V}\boldsymbol{\lambda}$$

- **POD modes**: $\xi_i(\boldsymbol{x}) = \frac{1}{N_t} \sum_{j=1}^{N_t} \boldsymbol{V}_{ji} \boldsymbol{u}_j(\boldsymbol{x})$
- **Reduced solution**: $\boldsymbol{u}^{ROM}(\boldsymbol{\mu}) = \sum_{i=0}^{N_r} u_i(\boldsymbol{\mu}) \xi_i(\boldsymbol{x})$
- **Galerkin projection**:

$$\left(a\left(\sum_{i=0}^{N_r} u_i(\boldsymbol{\mu}) \boldsymbol{\xi}_i \right), \boldsymbol{\xi}_j \right)_{L^2} = 0 \quad \text{for} \quad j = 1, \ldots, N_r$$

Reduced basis:
Every element of the space in terms of its own FEM base:

$$\boldsymbol{u}_{N_h}(\boldsymbol{\mu}) = \sum_{i=0}^{N_h} u_i(\boldsymbol{\mu}) \psi_i(\boldsymbol{x})$$

then we can evaluate RB (after Gram-Schmidt)

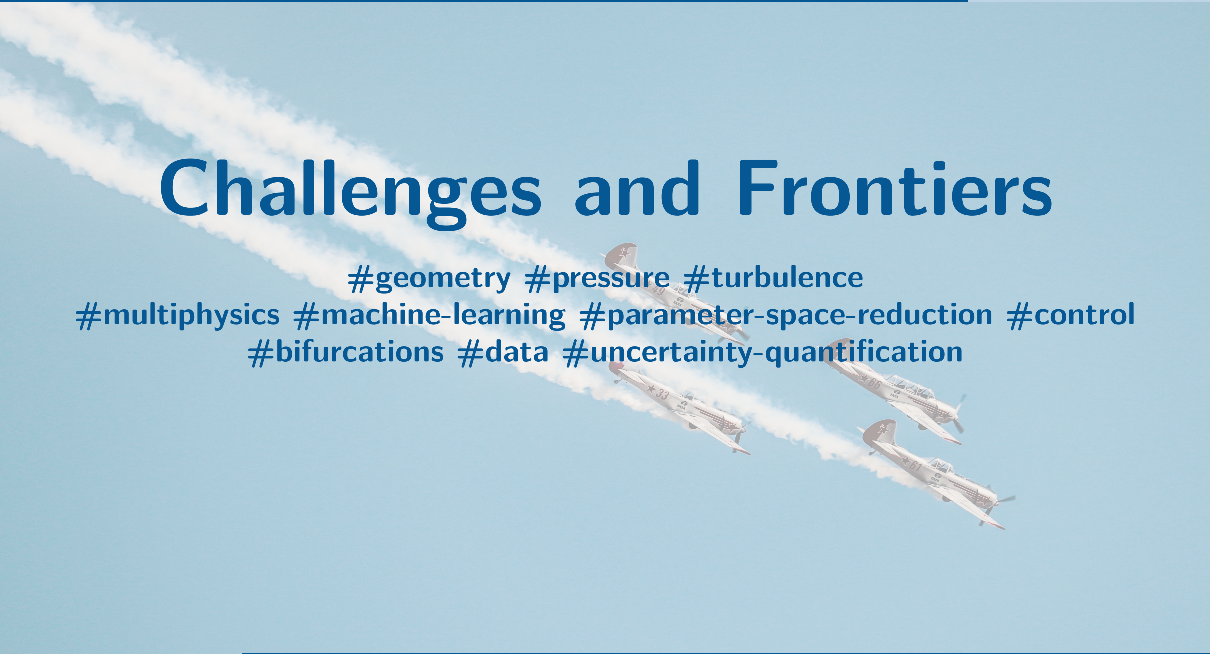
$$\boldsymbol{u}^{ROM}(\boldsymbol{\mu}) = \sum_{i=0}^{N_r} u_i(\boldsymbol{\mu}) \zeta_i(\boldsymbol{x})$$

where

$$\sum_{i=0}^{N_r} a\left(\zeta_i, \zeta_j; \mu \right) u_i^{N_r} = 0 \quad \text{for} \quad i = 1, \ldots, N_r$$

Reduced Order formulation: $\boldsymbol{A}^{ROM}(\boldsymbol{\mu})\boldsymbol{u}^{ROM}(\boldsymbol{\mu}) = 0,$ with $\mathbf{A}^{ROM} \in \mathbb{R}^{N_r} \times \mathbb{R}^{N_r}$

J. S. Hesthaven, G. Rozza, and B. Stamm., "Certified Reduced Basis Methods for Parametrized Partial Differential Equations", SpringerBriefs in Mathematics, Springer, 2015

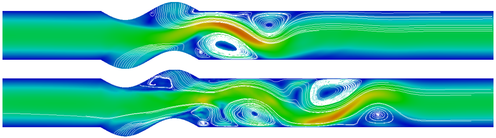


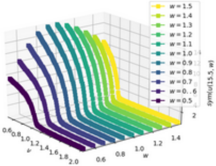
Challenges and Frontiers

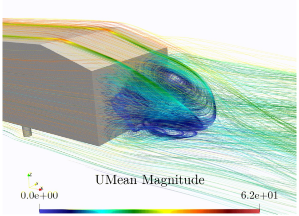
#geometry #pressure #turbulence
#multiphysics #machine-learning #parameter-space-reduction #control
#bifurcations #data #uncertainty-quantification

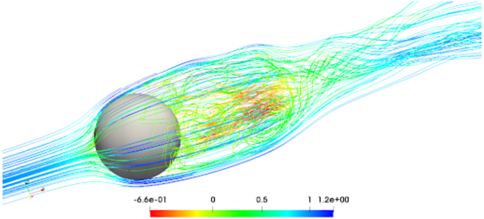
Strategic Fields of development for ROMs

- **Geometric Parametrization** (shape design)
- Increasing Reynolds number
- Improve **Pressure recovery** (accuracy)
- **Coupling** multi-physics
- **Automatic-learning** developments
- **Turbulence** (ROMs for RANS and LES)
- **Parameter space reduction**
- Flow **control** and data assimilation
- **Bifurcations** and flow stability









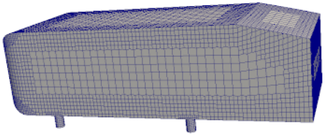
Gianluigi Rozza grozza@sissa.it

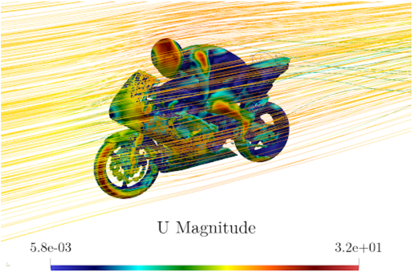
ROM challenges in CFD

Classical Discretization techniques:

FEM (Finite Element Method)	**FVM** (Finite Volume Method)

increasing Reynolds number →



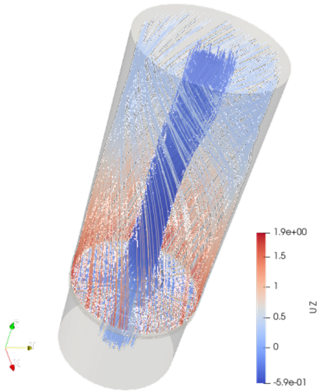


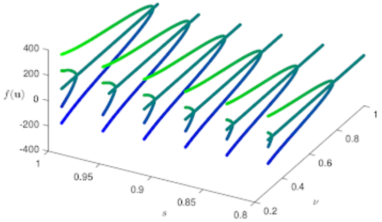
Key problems:

- **Stabilization issues** and fulfillment of *inf-sup* condition
  - stabilization approaches (SUPG, variational multi-scale approach)
  - SUP-ROM: addition of supremizer modes to enrich the velocity space
  - PPE-ROM: replacement of the continuity equation with the pressure Poisson equation
- **Turbulence treatment**
- Reliability of classical and reduced discretization methods in **real world applications**

Other options:

SEM (Spectral Element Method)	DG (Discontinuous Galerkin)





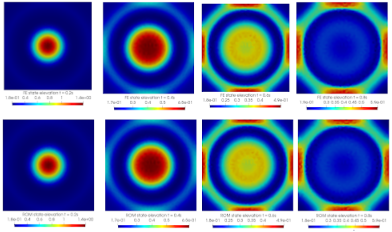
Key problems:

- Applications to **compressible flows**
- **Bifurcations** and study of flow stability
- Study of **multiphysics problems** (Fluid-Structure Interaction, heat transfer, ...)

Stabilization techniques for FEM-based ROM

FEM
(Finite Element Method)

- appropriate selection of velocity and pressure spaces to fulfill the **inf-sup condition** $(\mathbb{P}_k - \mathbb{P}_{k-1})$ [2] : supremizers
- spurious oscillation terms in **advection-dominated** problems
- introduction of stabilization methods, as **SUPG** (Streamline Upwind Petrov–Galerkin) for $\mathbb{P}_k - \mathbb{P}_k$ spaces, $k \geq 0$. OFFLINE-ONLINE stabilization.



[1]**What is the *inf-sup* condition?**

Consider the saddle-point problem:

Find u in V, p in Q such that,

$\forall$v in V and $\forall$ q in Q:

$$\begin{cases} a(u,v) + b(v,p) = \langle f, v \rangle \\ b(u,q) = \langle g, q \rangle . \end{cases}$$

The inf-sup condition is the sufficient condition for the **uniqueness** of the solution (u,p). It is defined as:

$$\inf_{q \in Q, q \neq 0} \sup_{v \in V, v \neq 0} \frac{b(v,q)}{\|v\|_V \|q\|_Q} \geq \beta,$$

$\beta \geq 0$.

G. Rozza, and K. Veroy (2007). On the stability of the reduced basis method for Stokes equations in parametrized domains. Computer methods in applied mechanics and engineering, 196(7), 1244-1260.

Stabilization techniques for FV- and POD-based ROM

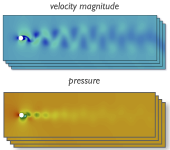
FVM (Finite Volume Method)

- **Hypothesis of POD-Galerkin ROMs**:

$$\mathbf{u}(\mathbf{x},t) \sim \sum_{i=1}^{N_u} a_i(t)\,\boldsymbol{\phi}_i(\mathbf{x})\,, \quad p(\mathbf{x},t) \sim \sum_{i=1}^{N_p} b_i(t)\,\chi_i(\mathbf{x})\,, \quad N_u, N_p \ll \text{ offline } \textbf{dofs}$$

- **Standard** approach:

Time snapshots



$\left[\mathbf{u}(\mathbf{x},t_1),\ldots,\mathbf{u}(\mathbf{x},t_{N_T})\right]$

$\left[p(\mathbf{x},t_1),\ldots,p(\mathbf{x},t_{N_T})\right]$

→ *Extraction of POD modes*

$(\boldsymbol{\phi}_i)_{i=1}^{N_u}$ velocity modes

$(\chi_i)_{i=1}^{N_p}$ pressure modes

→ *Vectors of coefficients*

$\mathbf{a}(t) = (a_i)_{i=1}^{N_u} = ?$

$\mathbf{b}(t) = (b_i)_{i=1}^{N_p} = ?$

- **Reduced system of ODEs**: $\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a},\mathbf{b}) \\ h(\mathbf{a}) = 0 \end{cases}$

- **Lack of accuracy** of standard ROMs → **Stabilized-ROMs**

- **Alternative velocity-pressure coupling** in the reduced system of ODEs:

FVM (Finite Volume Method)

SUP-ROM

- Enrichment of the velocity POD space with N_{sup} ***supremizer*** modes
- Fulfillment of the *inf-sup* condition when:

$$N_{sup} \geq N_p$$

$$\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}) \\ h(\mathbf{a}) = 0 \end{cases} \qquad \mathbf{a} = (a_i)_{i=1}^{r}, r = N_u + N_{sup}$$

PPE-ROM

- Replace the continuity equation with the ***Pressure Poisson Equation*** (PPE)

At the full order level:

$$\nabla \cdot \mathbf{u} = 0 \rightarrow \Delta p = -\nabla \cdot (\nabla \cdot (\mathbf{u} \otimes \mathbf{u}))$$

At the reduced order level:

$$\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}) \\ h_{PPE}(\mathbf{a}, \mathbf{b}) = 0 \end{cases}$$

G. Stabile, and G. Rozza, "Finite volume POD-Galerkin stabilised reduced order methods for the parametrised incompressible Navier–Stokes equations", Computers & Fluids 173 (2018): 273-284.

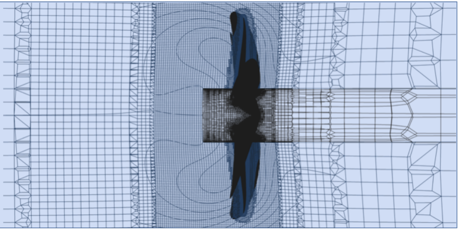
Turbulent Data-driven Stabilized-ROMs

#CFD #pressure #turbulence
#stabilizations #machine-learning

with Anna Ivagnes, Giovanni Stabile, Andrea Mola, Traian Iliescu

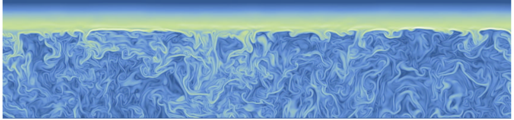
Why not Direct Numerical Simulation?

- *High* number of degrees of freedom
- *High* computational time
- Modeling *PDEs*



How to deal with turbulence?

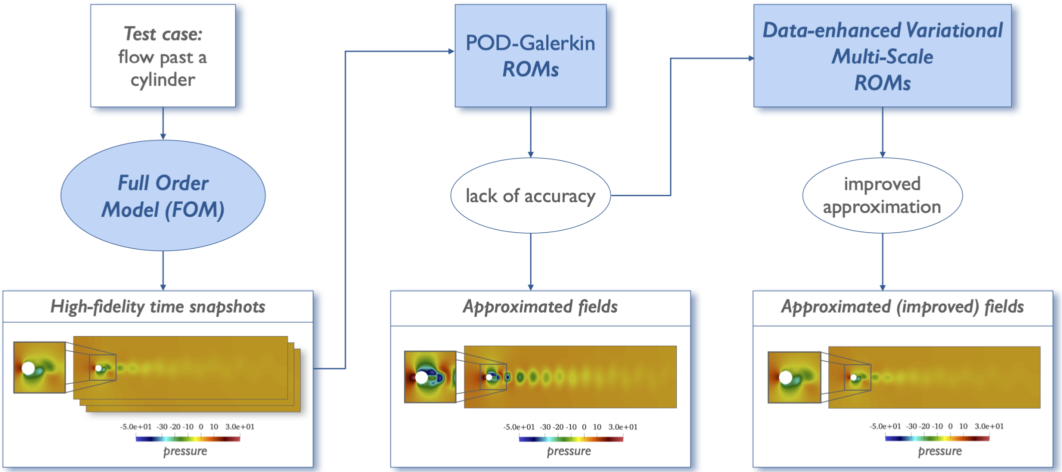
- Stabilization issues at high Reynolds' number
- Introduction of a *fictitious (eddy) viscosity*



Stabilization techniques for ROMs

- *Purely* data-driven approach
- *Physics-based* data-driven approach

Offline-online procedure



Purely data-driven ROM

LES-inspired idea:

to reintroduce the contribution of the neglected modes in ROMs

How:

extra correction terms

SUP-ROM

$$\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}) + \boldsymbol{\tau}_u(\mathbf{a}) \\ h(\mathbf{a}) = 0 \end{cases}$$

- ***Velocity correction:***

$$\boldsymbol{\tau}_u(\mathbf{a}) = \tilde{A}\mathbf{a} + \mathbf{a}^T \tilde{B}\mathbf{a}$$

- ***Operator:*** non-linear term

PPE-ROM

$$\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}) + \boldsymbol{\tau}_u(\mathbf{a}) \\ h_{PPE}(\mathbf{a}, \mathbf{b}) + \boldsymbol{\tau}_p(\mathbf{a}, \mathbf{b}) = 0 \end{cases}$$

- ***Velocity + pressure corrections:***

$$\begin{bmatrix} \boldsymbol{\tau}_u(\mathbf{a}, \mathbf{b}) \\ \boldsymbol{\tau}_u(\mathbf{a}, \mathbf{b}) \end{bmatrix} = \tilde{A}_p \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} + \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}^T \tilde{B}_p \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}$$

- ***Operators:*** non-linear term + different operators in PPE

A. Ivagnes, G. Stabile, A. Mola, G. Rozza and T. Iliescu, "Pressure Data-Driven Variational Multiscale Reduced Order Models", Journal of Computational Physics (2023) 111904.

Physics-based data-driven ROM

Idea:

to add the turbulence modeling in ROMs

How:

a ***reduced eddy viscosity field***

Procedure:

Extract the

eddy viscosity modes

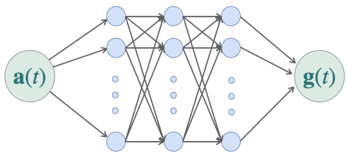
$$\left(\eta_i\right)_{i+1}^{N_{\nu_t}}$$

$$\nu_t \sim \sum_{i=1}^{N_{\nu_t}} g_i(t)\,\eta_i(\mathbf{x})$$

→

Compute $\mathbf{g}(t)$ through

a ***regression technique***



→

Integrate the model

into the ROMs

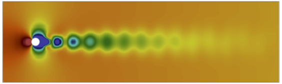
SUP-ROM $\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}, \mathbf{g}) \\ h(\mathbf{a}) = 0 \end{cases}$

PPE-ROM $\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}, \mathbf{g}) \\ h_{PPE}(\mathbf{a}, \mathbf{b}, \mathbf{g}) = 0 \end{cases}$

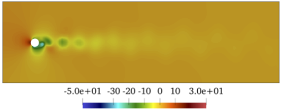
S. Hijazi, G. Stabile, A. Mola, and G. Rozza, "Data-driven POD-Galerkin reduced order model for turbulent flows." Journal of Computational Physics 416 (2020): 109513.

Results for **hybrid** formulation

Graphical results (*pressure field*)

	SUP-ROM	**PPE-ROM**
	$\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}, \mathbf{g}) + \boldsymbol{\tau}_u(\mathbf{a}) \\ h(\mathbf{a}) = 0 \end{cases}$	$\begin{cases} \dot{\mathbf{a}} = f(\mathbf{a}, \mathbf{b}, \mathbf{g}) + \boldsymbol{\tau}_u(\mathbf{a}) \\ h_{PPE}(\mathbf{a}, \mathbf{b}, \mathbf{g}) + \boldsymbol{\tau}_p(\mathbf{a}, \mathbf{b}) = 0 \end{cases}$
Standard ROMs		
Hybrid data-driven ROMs		

FOM



A. Ivagnes, G. Stabile, A. Mola, G. Rozza and T. Iliescu, "Hybrid data-driven closure strategies for reduced order modeling", accepted for publication in Journal of Applied Mathematics and Computation (2023).

LES-ROM for incompressible flows

#turbulent flows #large eddy simulation #POD #data-driven

with Michele Girfoglio and Annalisa Quaini

High-fidelity formulation for a LES model: **Offline stage**

We consider a fixed domain $\Omega \subset \mathbb{R}^D$ with $D = 2, 3$ over a time interval of interest $(t_0,\ T) \subset \mathbb{R}^+$. The flow is described by the **Leray** model:

$$
\begin{aligned}
\rho\, \partial_t \mathbf{u} + \rho\, \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - 2\mu \Delta \mathbf{u} + \nabla p = 0 \quad & \text{in } \Omega \times (t_0, T), \\
\nabla \cdot \mathbf{u} = 0 \quad & \text{in } \Omega \times (t_0, T), \\
-\delta^2 \nabla \cdot (a \nabla \overline{\mathbf{u}}) + \overline{\mathbf{u}} + \nabla \lambda = \mathbf{u} \quad & \text{in } \Omega \times (t_0, T), \\
\nabla \cdot \overline{\mathbf{u}} = 0 \quad & \text{in } \Omega \times (t_0, T),
\end{aligned}
$$

where $\overline{\mathbf{u}}$ is the filtered velocity, λ is a Lagrange multiplier to enforce the incompressibility constraint and a is the so-called *indicator function* which is ≈ 0 where the velocity $\mathbf{u}$ does not need regularization and ≈ 1 where the velocity $\mathbf{u}$ does need regularization.

Collection of **high-fidelity snapshots** with big number of degrees of freedom → **Dimensionality reduction**: **POD** with Galerkin approach — ITHACA-FV library → Extraction of velocity, pressure and indicator function modes

A data-driven POD-Galerkin method: **Online stage**

Basic idea:
Exploiting a **traditional projection method for the computation of the reduced velocity and pressure fields**, while we use a **data-driven technique based on Radial Basis Functions to compute the reduced coefficients of the indicator function field**.

Motivation:

* the use of a hybrid approach is accurate and partially non-intrusive;
* unique computational pipeline for the development of efficient ROMs for turbulent flows (no matter if modeled by LES or RANS).

Main novelties:

* The use within the **Evolve-Filter-Relax algorithm** of a **nonlinear deconvolution-based indicator function**;
* The use of a **filtering approach** both in the **offline** and **online** stages;
* The computation of the pressure field at ROM level;
* The use of the **finite volume method for the space discretization**. Most ROM spatial discretizations utilize finite element or other Galerkin formulations. However, many commercial codes are based on FV methods. Thus, **the combination of ROM and FV methods is appealing for practical applications**.

Illustrative results for a 2D flow past a cylinder

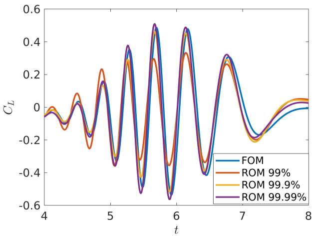


Figure: Time evolution of the lift coefficient computed by FOM and ROM.

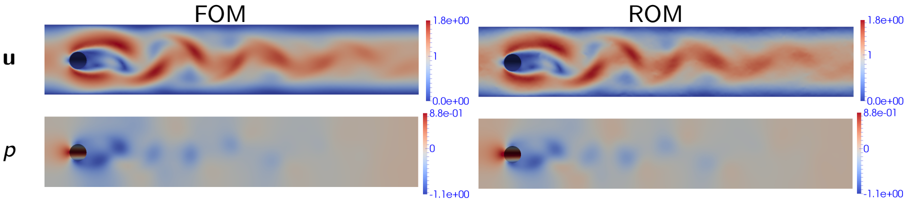


Figure: Velocity and pressure fields computed by FOM and ROM at $t = 5.5$.

Illustrative results for a 3D flow past a cylinder

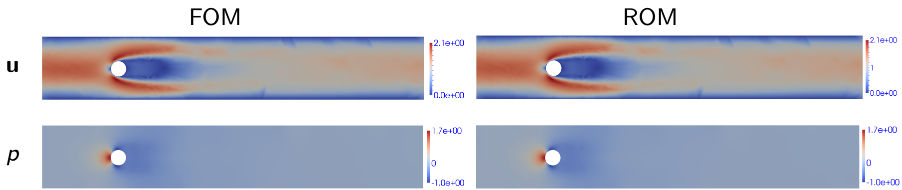


Figure: Velocity, pressure and indicator function fields computed by FOM and ROM on the midsection at $t = 5.5$.

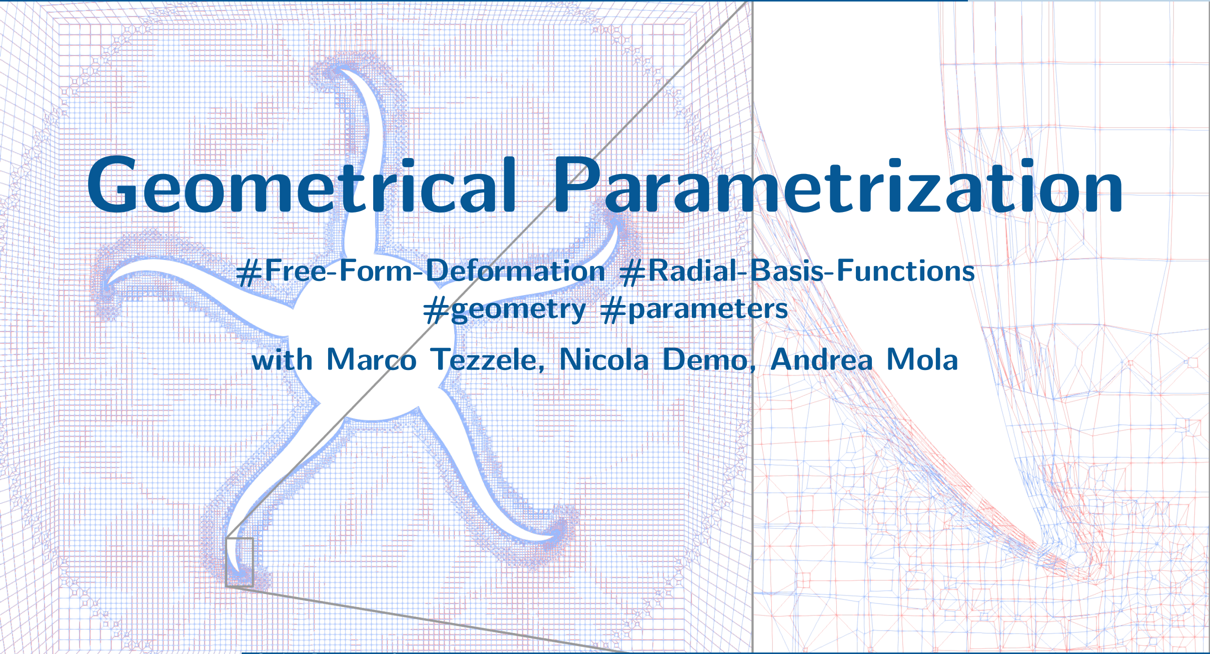
Speed-up ≈ 230

M. Girfoglio, A. Quaini, and G. Rozza, "A Finite Volume approximation of the Navier-Stokes equations with nonlinear filtering stabilization", Computers & Fluids, 187:27-45, 2019. doi: 10.1016/j.compfluid.2019.05.001.

M. Girfoglio, A. Quaini, and G. Rozza, "A POD-Galerkin reduced order model for a LES filtering approach", Journal of Computational Physics, 436:110260, 2021. doi: 10.1016/j.jcp.2021.110260.

M. Girfoglio, A. Quaini, and G. Rozza, "Pressure Stabilization Strategies for a LES Filtering Reduced Order Model", Fluids, 6, 2021. doi: doi.org/10.3390/fluids6090302

M. Girfoglio, A. Quaini, and G. Rozza, "A hybrid projection/data-driven reduced order model for the Navier-Stokes equations with nonlinear filtering stabilization", Journal of Computational Physics, 486, 2023. doi: doi.org/10.1016/j.jcp.2023.112127

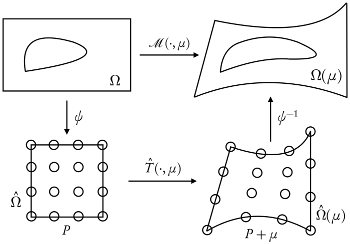


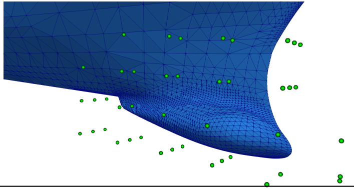
Geometrical Parametrization

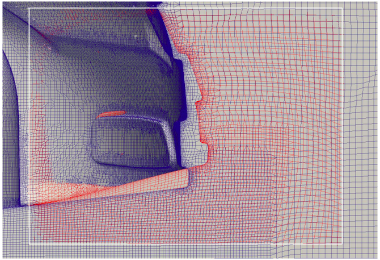
#Free-Form-Deformation #Radial-Basis-Functions #geometry #parameters

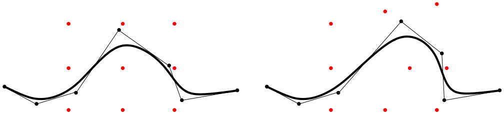
with Marco Tezzele, Nicola Demo, Andrea Mola

Geometrical parametrisation: Free form deformation





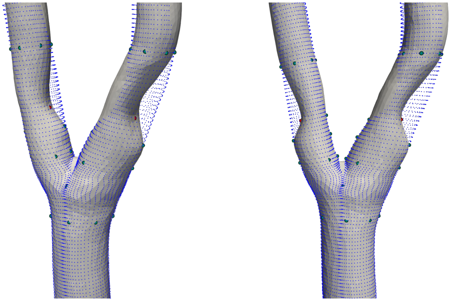


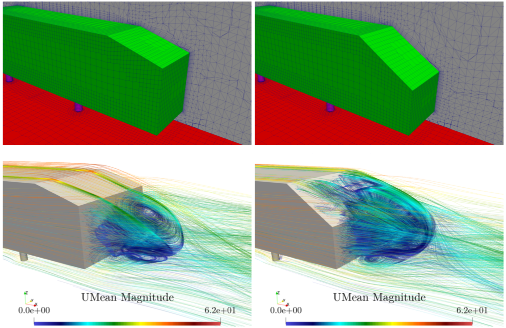


[1]**F. Salmoiraghi, A. Scardigli, H. Telib and G. Rozza** (2018) *Free-form deformation, mesh morphing and reduced-order methods: enablers for efficient aerodynamic shape optimisation*. International Journal of Computational Fluid Dynamics, 32:4-5, 2018

[2]**M. Tezzele, F. Salmoiraghi, A. Mola, and G. Rozza**. *Dimension reduction in heterogeneous parametric spaces with application to naval engineering shape design problems*. Advanced Modeling and Simulation in Engineering Sciences, 5(1):25, Sep 2018

Geometrical parametrisation: Radial basis functions interpolation



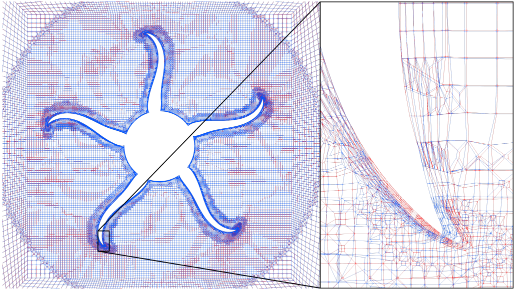


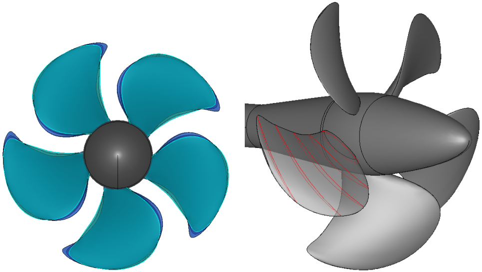
[1] **M. Tezzele, F. Ballarin, and G. Rozza**. *Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD- Galerkin methods*. In D. Boffi, L. F. Pavarino, G. Rozza, S. Scacchi, and C. Vergara, editors, Mathematical and Numerical Modeling of the Cardiovascular System and Applications, volume 16 of SEMA-SIMAI Series, pages 185–207. Springer International Publishing, 2018.

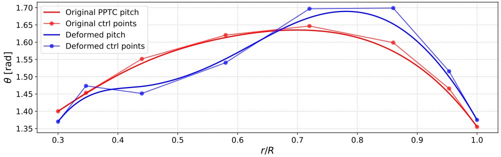
[2] **M. Zancanaro, M. Mrosek, G. Stabile, C. Othmer, and G. Rozza**, *Hybrid Neural Network Reduced Order Modelling for Turbulent Flows with Geometric Parameters*, Fluids, 6, 2021

[3] **N. Demo, M. Tezzele, A. Mola, and G. Rozza**. *Hull Shape Design Optimization with Parameter Space and Model Reductions, and Self-Learning Mesh Morphing*. Journal of Marine Science and Engineering, 9(2):185, 2021.

Geometrical parametrisation: Object specific deformations







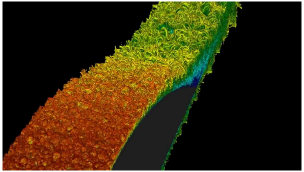
[1] **A. Mola, N. Demo, M. Tezzele, and G. Rozza**. *Geometrical Parameterization and Morphing Techniques with Applications*. In G. Rozza, G. Stabile, and F. Ballarin, editors, Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics, CSE Vol.27, chapter 17. SIAM Press, 2022

ROMs for Turbulent flows with Geometrical Parametrization

#turbulence #Navier-Stokes #multiphysics #CFD #parameter-space-reduction #vortex shedding

with Matteo Zancanaro, Markus Mrosek and Giovanni Stabile

ROM for turbulent flows



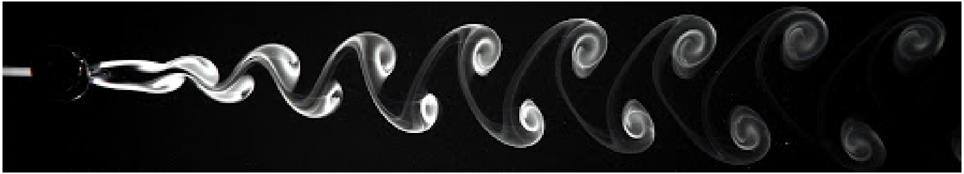
Why not a Direct Numerical Simulation?

- **huge dimension** of the problem is required;
- **computational time** gets unaffordable;
- for many applications such an accuracy is **not needed**.

Involved conservation laws: Incompressible Navier–Stokes Equations

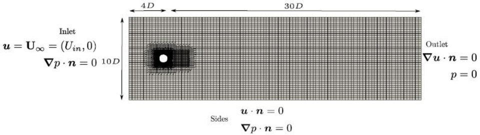
$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} = -\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) + \nabla \cdot \nu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \nabla p & \text{in } \Omega \times [0, T], \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \times [0, T]. \end{cases}$$

where $\nu = \mu / \rho$ is the kinematic viscosity.



Test case: **turbulent flow** around a **circular cylinder** with $Re = 5 \times 10^4$.
The high-fidelity simulations are held in **OpenFOAM**, using:

* **RANS** (Reynolds Averaged Navier-Stokes) approach;
* **FVM** (Finite Volume Method) for space discretization.



RANS formulation:

$$\begin{cases} \nabla \cdot (\overline{\boldsymbol{u}} \otimes \overline{\boldsymbol{u}}) - (\nu + \nu_t)\, \nabla^2 \overline{\boldsymbol{u}} + \nabla \overline{p} + \dfrac{2}{3} \nabla k = 0 \\ \nabla \cdot \overline{\boldsymbol{u}} = 0, \end{cases}$$

where ν_t stands for the eddy viscosity while k represents the turbulent kinetic energy.

High-fidelity snapshots:
$[\mathbf{u}_1, \dots, \mathbf{u}_{N_T}]$, $[p_1, \dots, p_{N_T}]$
with big number of degrees of freedom

→

Dimensionality reduction:
POD with Galerkin approach

ITHACA - FV

→

Extraction of
velocity modes $(\varphi_i)_{i=1}^{N_u^h}$
and
pressure modes $(\chi_j)_{i=j}^{N_p^h}$

Standard Galerkin-ROM framework: **Online stage**

The **standard ROM** framework is followed:

* pick a **reduced** number of modes r for velocity and q for pressure;
* express the **reduced fields** as:

$$\mathbf{u}_r = \sum_{i=1}^{r} a_i \, \boldsymbol{\varphi}_i, \; p_r = \sum_{j=1}^{q} b_j \, \chi_j \longrightarrow$$

Unknowns:
coefficient vectors
$\mathbf{a} = (a_i)_{i=1}^{r}$ and $\mathbf{b} = (b_j)_{j=1}^{q}$

* project the discretized NSE onto the reduced space, with two **velocity-pressure coupling** techniques and solve the **dynamical systems**:

SUP-ROM (supremizer approach)

$$\begin{cases} \dot{\mathbf{a}} = \mathbf{f}(\mathbf{a}, \mathbf{b}), \\ \mathbf{h}(\mathbf{a}) = \mathbf{0}. \end{cases}$$

* addition of supremizer modes to avoid stability issues: $r = N_u + N_{sup}$.

PPE-ROM (Pressure Poisson Equation approach)

$$\begin{cases} \dot{\mathbf{a}} = \mathbf{f}(\mathbf{a}, \mathbf{b}), \\ \mathbf{h}_{\mathrm{PPE}}(\mathbf{a}, \mathbf{b}) = \mathbf{0}. \end{cases}$$

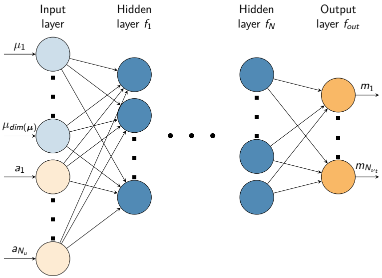
* continuity equation replaced by the PPE.

The number of modes belongs to the **marginally-resolved** regime: modes are enough to represent the underlying dynamics, but **the standard ROM yields inaccurate results**.

G. Stabile, and G. Rozza, "Finite volume POD-Galerkin stabilised reduced order methods for the parametrised incompressible Navier–Stokes equations", Computers & Fluids 173 (2018): 273-284.

Turbulent flows - Turbulence treatment in a **parametric setting**

The reconstruction of the **eddy viscosity field** can be done with a fully-connected **neural network** [2].



Reduced eddy viscosity field:
$\nu_{t\,r} = \sum_{i=1}^{N_{\nu_t}} m_i(\boldsymbol{x})\zeta_i(\boldsymbol{\mu})$, where:

* $\mathbf{m} = (m_i)_{i=1}^{N_{\nu_t}}$ is the eddy viscosity coefficient vector;
* $(\zeta_i)_{i=1}^{N_{\nu_t}}$ are the eddy viscosity modes.

Mapping from known modes:

$$\mathcal{F} : \mathbb{R}^{dim(\boldsymbol{\mu})+N_u} \to \mathbb{R}^{N_{\nu_t}}, \quad \mathcal{F}(\boldsymbol{\mu}, \overline{\boldsymbol{a}}(\boldsymbol{\mu})) = \boldsymbol{m}$$

Neural network mapping:

$$\tilde{\boldsymbol{m}} = \mathcal{F}_{network}(\boldsymbol{\mu}, \overline{\boldsymbol{a}}(\boldsymbol{\mu})), \text{ with } \mathcal{F}_{network} \text{ regression map}$$

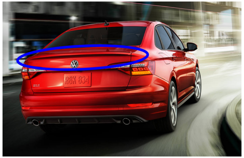
Loss function of the neural network:

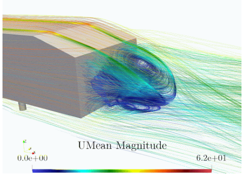
$$\mathcal{L} = \sum_{i=1}^{N_{\nu_t}} ||\boldsymbol{m}_i - \tilde{\boldsymbol{m}}_i||_{L^2}$$

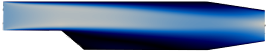
[2] **Zancanaro M., Mrosek M., Stabile G., Othmer C., Rozza G.**, (2021), *Hybrid neural network reduced order modelling for turbulent flows with geometric parameters*, MDPI-Fluids

Turbulent flows - Geometrical parametrization

Proposed test case: **back step** channel where the step is constructed as a **moving boundary** so that the slop β can be varied.



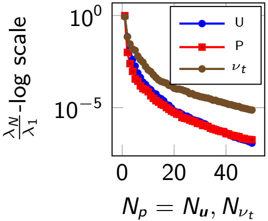


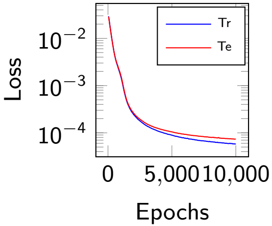


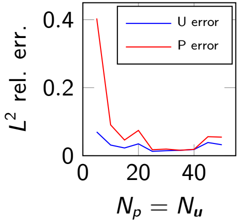
Data for the problem:

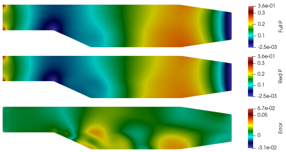
- Slop $\beta \in [0^\circ, 75^\circ]$
- $\boldsymbol{u}_x^{inlet} = 1\,\mathrm{m\,s^{-1}}$;
- $Re = \frac{u_x^{inlet} L}{\nu} = 9 \times 10^3$;
- $N_u = N_p = 35$;
- $N_{\nu_t} = 25$;
- **Activation function**: ReLu, 10^4 epochs;
- $N_{off} = 50$;
- $\Delta = 50$;
- $\beta_{on} = 65^\circ$.

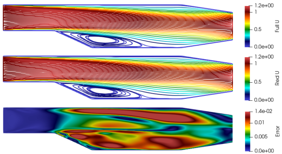
Turbulent flows - Geometrical parametrization [3] [4]

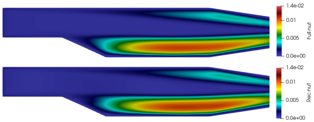












[3] **Zancanaro M., Mrosek M., Stabile G., Othmer C., Rozza G.**, (2021), *Hybrid neural network reduced order modelling for turbulent flows with geometric parameters*, MDPI-Fluids

[4] **Stabile G., Zancanaro M., Rozza G.**, (2020), *Efficient Geometrical Parametrization for Finite-Volume based Reduced Order Methods*, International Journal for Numerical Methods in Engineering.

ROMs for Compressible flows

#compressible #Mach #shocks
#CFD #geometrical-parametrization

with Matteo Zancanaro and Giovanni Stabile

Source of image: NASA

Compressible flows - The problem

What is the problem characterized by?

* Mach number > 0.3;
* **varying density field**;
* thermodynamics for energy evolution;
* no shocks;
* **high turbulent fluctuations**.

Involved conservation laws: **Favre averaged Navier-Stokes equations**

$$\begin{cases} \nabla \cdot (\overline{\rho}\tilde{\boldsymbol{u}}) = 0 \\ \nabla \cdot [\overline{\rho}\tilde{\boldsymbol{u}} \otimes \tilde{\boldsymbol{u}} - \tilde{\boldsymbol{\tau}}_{turb} - \tilde{\boldsymbol{\tau}} + \overline{p}\boldsymbol{I}] = 0 \\ \nabla \cdot \left[\overline{\rho}\tilde{\boldsymbol{u}}\left(\tilde{e} + \dfrac{\tilde{\boldsymbol{u}} \cdot \tilde{\boldsymbol{u}}}{2}\right) - \dfrac{C_p}{C_v}\dfrac{\mu}{Pr}\nabla\tilde{e} - \dfrac{C_p}{C_v}\dfrac{\mu_t}{Pr_t}\nabla\tilde{e} + \overline{p}\tilde{\boldsymbol{u}}\right] = 0 \end{cases}$$

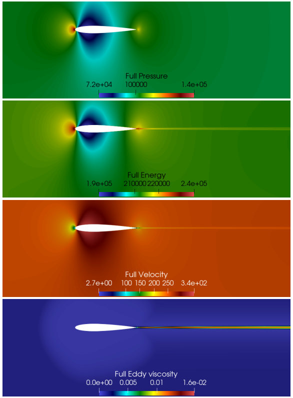
Gianluigi Rozza grozza@sissa.it

Compressible flows - Physical and Geometrical parametrization

Proposed test case: flow around a **NACA**0012 airfoil where characteristics of the airfoil or the flow can be changed leading to either Physical or Geometrical parametrization.

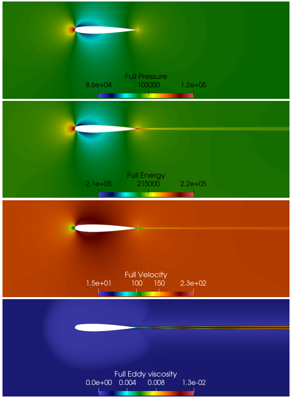
Physical Parametrization

* Mach $= 0.73$;
* $Re \in 2.92 \times [10^4, 10^7]$;



Geometrical Parametrization

* Mach $= 0.5$;
* $Re \in 1.14 \times 10^7$.



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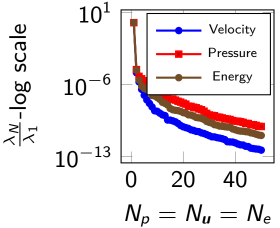
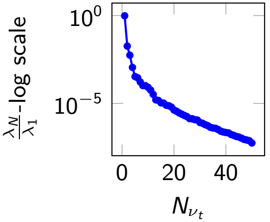
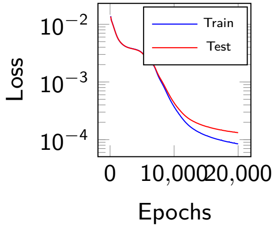
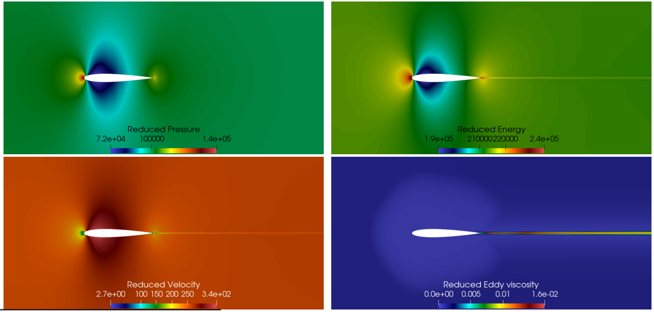
Compressible flows - Physical parametrization [5]



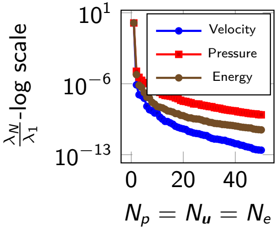


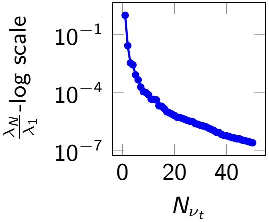


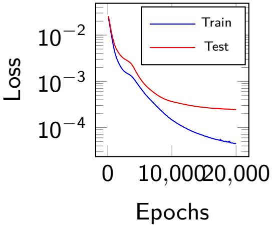


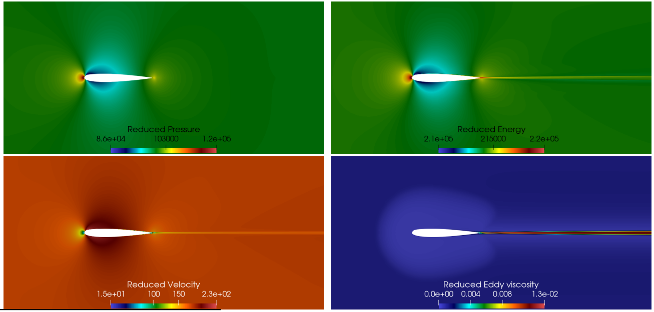
[5] **M. Zancanaro, G. Stabile, and G. Rozza**, (2022), *Reduced Order Models for compressible flow in a Finite-Volume framework based on segregated solvers*

Compressible flows - Geometrical parametrization [6]







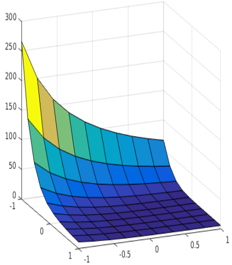


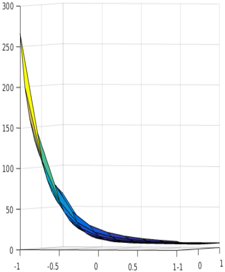
[6] **M. Zancanaro, G. Stabile, and G. Rozza**, (2022), *Reduced Order Models for compressible flow in a Finite-Volume framework based on segregated solvers*

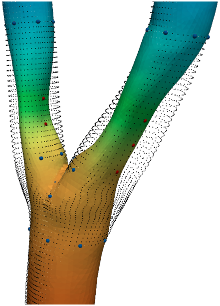
Shape parametrization # Active subspaces # POD-Galerkin # Carotid arteries

Combined parameter and model reduction with shape parametrization by active subspaces and POD-Galerkin

with Marco Tezzele







Active subspaces property

In many cases the dimension of the parametrised problem is only artificially high

- Active subspaces property identifies a set of important directions in the space of all inputs.

$$f : \mathbb{R}^m \to \mathbb{R} \qquad \mathbf{x} \in \mathbb{R}^m$$

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

$$\mathbf{C} = \mathbf{W} \mathbf{\Lambda} \mathbf{W}^T$$

f is a scalar function that takes as arguments the parameters x

C is the uncentered covariance matrix of the gradients of f, symmetric, positive semidefinite

E is the expected value and rho a probability density function

- We define the active subspace to be the range of the **first n eigenvectors** of W

$$\mathbf{W} = [\mathbf{W_1} \quad \mathbf{W_2}] \in \mathbb{M}^{m \times m} \qquad \mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda_1} & \\ & \mathbf{\Lambda_2} \end{bmatrix}$$

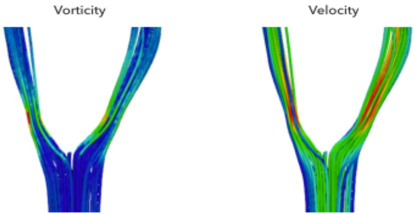
- With the basis identified, we can map forward to the active subspace. So **y is the active variable** and z the inactive one. The **surrogate model** g is used to approximate f

$$\mathbf{y} = \mathbf{W}_1^{\mathbf{T}} \mathbf{x} \in \mathbb{R}^n \qquad \mathbf{z} = \mathbf{W}_2^{\mathbf{T}} \mathbf{x} \in \mathbb{R}^{m-n} \qquad f(\mathbf{x}) \approx g(\mathbf{W}_1^{\mathbf{T}} \mathbf{x}) = g(\mathbf{y})$$

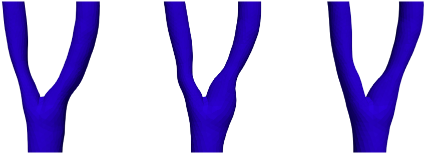
Constantine, Active subspaces: Emerging ideas for dimension reduction in parameter studies, SIAM, 2015.

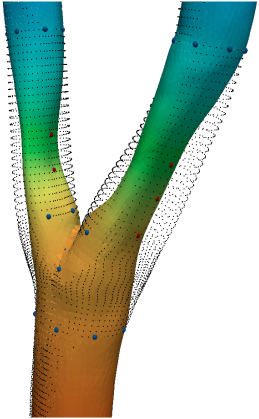
Flow across parametrised carotid bifurcations

- Vessels geometry strongly influences hemodynamics behaviour.
- The output function is the relative pressure drop of the two branches, computing the integral of the pressure on selected sections.



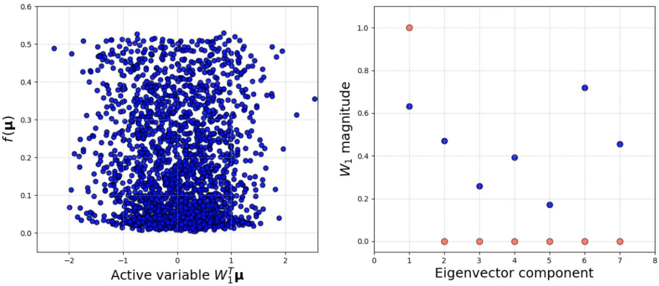
- We deform the carotid after the bifurcation moving 10 RBF control points (in red) solving an interpolation system.





Deformed carotid with the deforming control points (red) and the undeformed state (black)

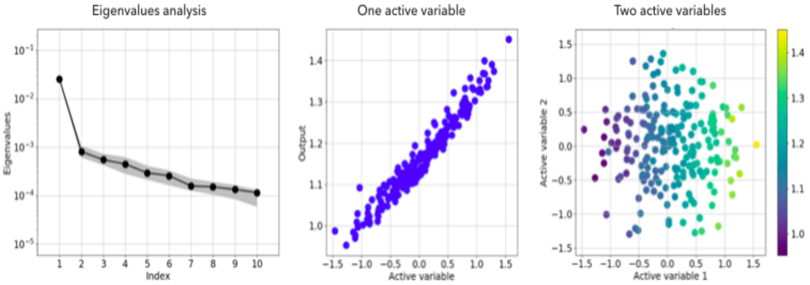
Active Subspaces - A quadratic example



M. Tezzele, F. Ballarin and G. Rozza "Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD-Galerkin methods", *Mathematical and Numerical Modeling of the Cardiovascular System and Applications*, 2018.
M. Tezzele, F. Salmoiraghi, A. Mola, G. Rozza. "Dimension reduction in heterogeneous parametric spaces with application to naval engineering shape design problems", Advanced Modeling and Simulation in Engineering Sciences, 2018.

Spectral analysis

- 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: 500:1.

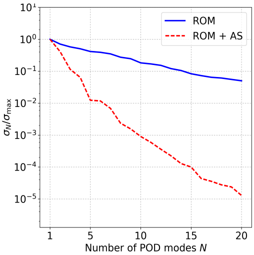


Tezzele, Ballarin, and Rozza, Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD-Galerkin methods. Contributed chapter SEMA/SIMAI 2018.

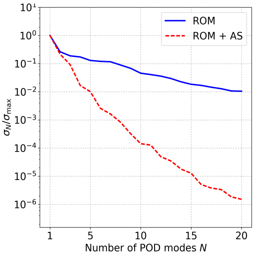
POD analysis

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

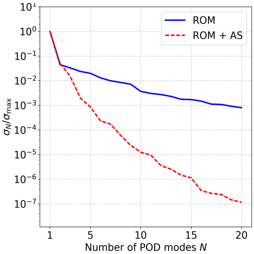
Velocity



Supremizers

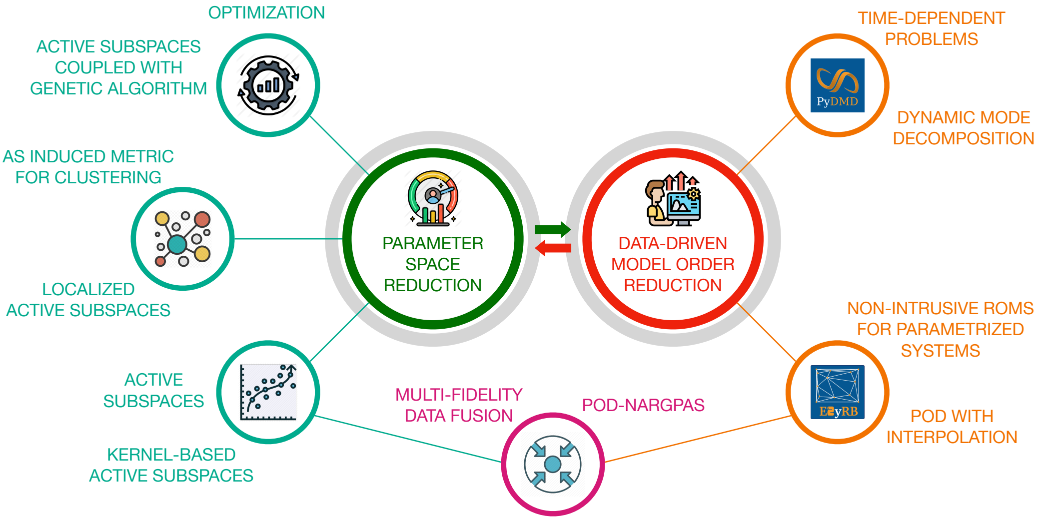


Pressure

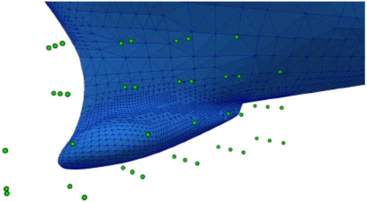


- The standard approach presents a slower decay, meaning that it has to deal with a considerably larger solution manifold.
- The combined methodology is able to reach relative errors which are up to one order of magnitude smaller when compared to the standard one, for both velocity and pressure when $N = 20$.

The many aspects of parameter space reduction



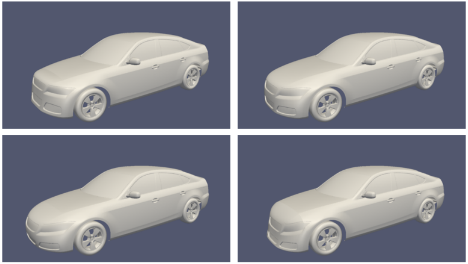
#GeometricalMorphing #Industrial #applications #FFD
A full Monolithic data-driven ROMs computational for FSI problems pipeline
with Marco Tezzele, Nicola Demo, Andrea Mola



PyGeM: Python Geometrical Morphing

- PyGeM is a python library using Free Form Deformation, Inverse Distance Weighting, and Radial Basis Function interpolation technique to parametrize and morph complex geometries. It is developed by F. Salmoiraghi, N. Demo, and M. Tezzele
- The main focus of PyGeM is to interact with the major industrial file formats used for CAD management. Since it has to integrate itself in the industrial workflow we have chosen python

Morphing of the bumper using an OpenFOAM file. DrivAer model.



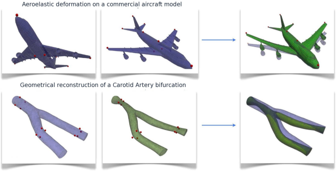
- It allows to handle:
  - Computer Aided Design files (.iges, .step and .stl)
  - Mesh files (.unv and OpenFOAM)
  - Output files (.vtk)

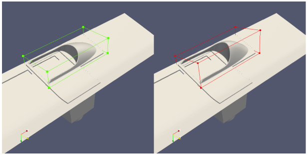
PyGeM on Github: github.com/mathLab/PyGeM

Efficient and accurate geometrical parametrization techniques

- At the state of the art free-form parametrization techniques for geometries are receiving a growing interest, in view of strong integration with CAD tools, as well as for design and shape optimization
- Extending isogeometric analysis (IGA) for viscous f ows in the reduced basis context

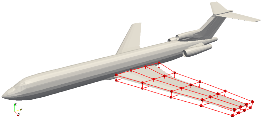
$$T(\underline{x}, \mu) : \Omega \to \Omega_0(\mu)$$

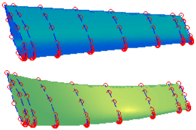




Underwater Blue Efficiency

MONTECARLOYACHTS





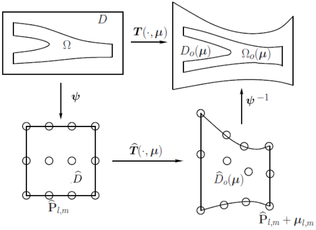
In collaboration with: F. Salmoiraghi, F. Ballarin, L. Heltai, A. Mola, M. Tezzele, N. Demo (SISSA), H. Telib, A. Scardigli (Optimad-PoliTo), D. Forti (EPFL)

Tool for the automatic shape parametrization

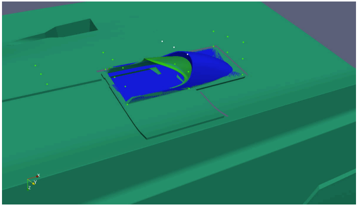
1. Mapping the physical domain to the reference one: ψ

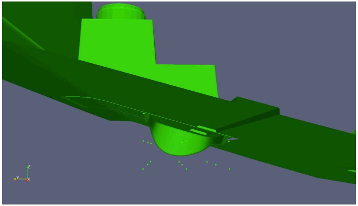
2. Moving some control points to deform the lattice: $\hat{T}$

3. Mapping back to the physical domain: ψ^{-1}



FFD: composition of the three maps $$T(\cdot,\mu) = (\psi^{-1} \circ \hat{T} \circ \psi)(\cdot,\mu)$$



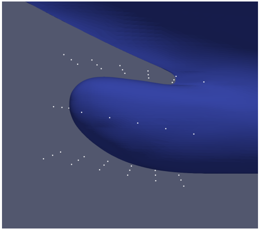


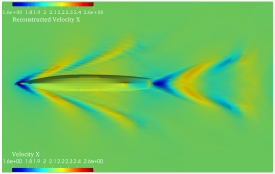
Reduced Order Model for industrial shape problems

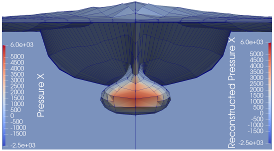
original hull → FFD → FV → DMD → PODI → OPT → optimized hull

In collaboration with Fincantieri, leader in cruise ship manifacturing, we developed an innovative pipeline involving **data-driven** reduced order modeling techniques for shape optimization in naval problems.

- **Shape parametrization** (FFD)
- **Proper orthogonal decomposition with interpolation**
- **Dynamic mode decomposition**







PyGeM EZyRB PyDMD

FINCANTIERI

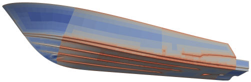
UNIONE EUROPEA
Fondo Europeo di Sviluppo Regionale

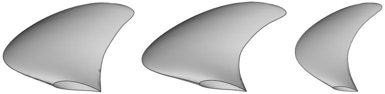
REGIONE AUTONOMA FRIULI VENEZIA GIULIA

FSE FRIULI VENEZIA GIULIA POR 2014 2020

Reduced Order Model for industrial shape problems

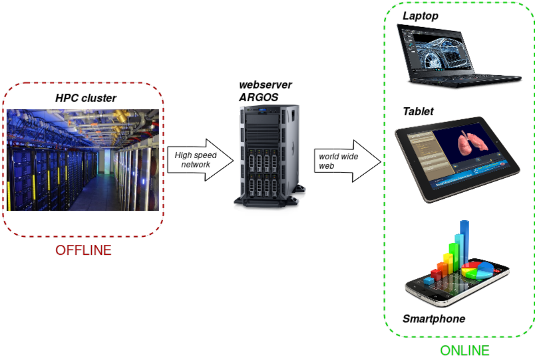
- **POR FESR: SOPHYA** the main goal of the project is to **improve planing yacht** hulls the performance in **non-calm sea** conditions. A set of specific methodologies have been developed to be able to **parameterize the hull** geometry and carry out a **shape optimization** campaign based both on high fidelity **RANS** and non-intrusive **ROM** simulations.
- **POR FESR: PRELICA** the main goal of the project is to **improve ship propeller** performance both in terms of **thrust** and **acoustic emissions**. A specific python package (**BladeX**) has been developed to generate **parametrized propeller** geometries. The optimal propeller shape has been identified making use of both high order **LES** and non-intrusive **ROM** hydroacoustic simulations.





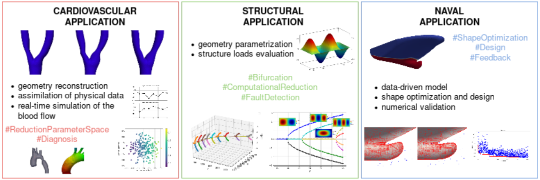
Vision and Perspective: to real-time computing

Model order reduction for web server: from biomedical to naval applications



CSE-Apps

- HPC, data science
- Web computing
- Digital twin
- 3D printing
- SMACT Industry4.0



Applications of Machine Learning

#AI #PINNs #DL #AE

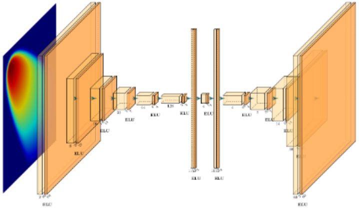
with Dario Coscia, Laura Meneghetti, Nicola Demo, Guglielmo Padula, Isabella Carla Gonnella, Anna Ivanes Francesco Romor, Maria Strazzullo and Giovanni Stabile

Artificial Intelligence: Deep Learning for enhancing Model Order Reduction

Artificial Intelligence can **enhance** classical ROM techniques for **Computational Fluid Dynamics**.

Enhancing data-driven reduction methods

- Approximation in Reduced Order Model (POD-NN, AE-NN)
- Automatic preprocess data for **dominant advection models**
- Auto-encoders for **dimensionality reduction** and **manifold learning**
- Reduction in **wide parameter space** by means of deep learning **parameter domain decomposition**



I. Gonnella, M. W. Hess, G. Stabile, and G. Rozza, (2023). " A two stages Deep Learning Architecture for Model Reduction of Parametric Time-Dependent Problems." arXiv preprint arXiv:2301.09926.

F. Romor, G. Stabile, and G. Rozza, (2023). "Non-linear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method." **J**ournal **S**cientific **C**omputing.

D. Papapicco, N. Demo, M. Girfoglio, G. Stabile, and G. Rozza, (2022). "The Neural Network shifted-proper orthogonal decomposition: A machine learning approach for non-linear reduction of hyperbolic equations.", accepted for **C**omputer **M**ethods in **A**pplied **M**echanics and **E**ngineering.

Artificial Intelligence: Solving Differential Equations with Deep Learning

Deep Learning can be a powerful tool for **solving Differential Equation** with **little data**

Physics-Informed Neural Networks

- Solving PDEs by **including physical laws and symmetries** in the Neural Network

Deep Operator Learning

- Approximate **PDEs operators** leveraging neural networks
- Data-driven, with possibility to make it physics-informed

PINA: a `python` package for differential equation modelling using deep learning.
`https://github.com/mathLab/PINA`

D. Coscia, A. Ivagnes, N. Demo, and G. Rozza (2023). "Physics-Informed Neural networks for Advanced modeling.", accepted for **J**ournal of **O**pen **S**ource **S**oftware.

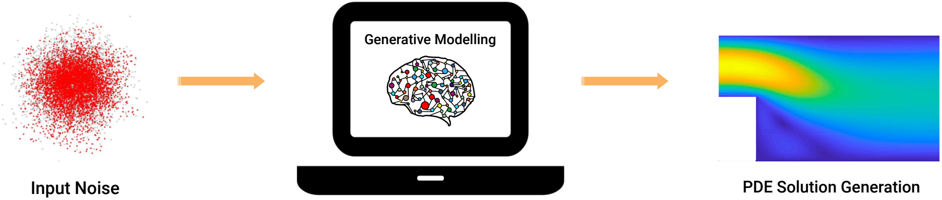
N. Demo, M. Strazzullo, and G. Rozza (2023). "An extended physics informed neural network for preliminary analysis of parametric optimal control problems.", accepted for **C**omputers **A**nd **M**athematics **W**ith **A**pplications.

N. Demo, M. Tezzele, and G. Rozza (2023). "A DeepONet multi-fidelity approach for residual learning in reduced order modeling.", arXiv preprint arXiv:2302.12682.

Deep Generative models leverage deep learning to generate **new data** that captures the intrinsic characteristics of the original ones.

Generative models as reduction technique

- **Generation of differential equation solutions** for parametric/time-dependent problems
- **Optimize meshes** by preserving the structural properties and generating new ones
- **Uncertainty Quantification** already integrated given the probabilistic approach
- **Upsampling** high fidelity solution databases only **data-driven**

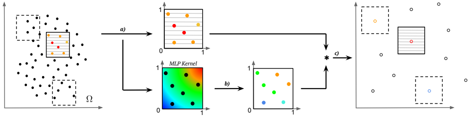


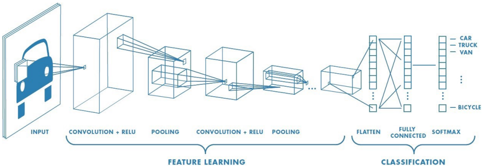
Artificial Intelligence: Reducing Neural Network Architectures with Machine Learning

Standard reduced order techniques can be applied to **compress** big neural network architectures

Continuous Convolutional Filter

- CNN working for **unstructured domains**
- Avoid computational burden of GNN





Compressing CNNs

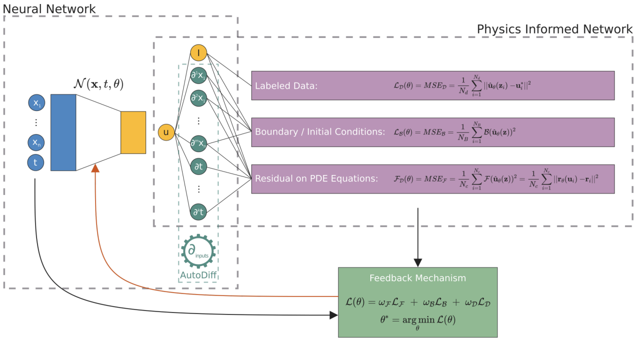
- **Parameter reduction** for CNNs architectures
- Reducing inference time and computational storage

D. Coscia, L. Meneghetti, N. Demo, G. Stabile, & G. Rozza. (2022). A Continuous Convolutional Trainable Filter for Modelling Unstructured Data. Computational Mechanics, Springer.

L. Meneghetti, N. Demo, and G. Rozza (2023). "A Dimensionality Reduction Approach for Convolutional Neural Networks." **AP**plied **IN**telligence, Springer.

Artificial Intelligence: Injecting Physical Laws in Neural Networks

Physics Informed Neural Networks solve differential equation by injecting the physics in the learning process. The PINN's final objective is to minimize the differential equation residuals.

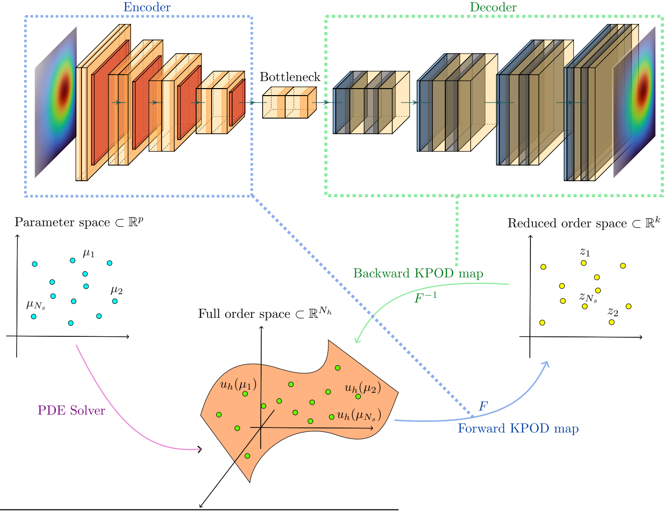


PINA: a python package for differential equation modelling using deep learning.
`https://github.com/mathLab/PINA`

D. Coscia, A. Ivagnes, N. Demo, and G. Rozza (2023). "Physics-Informed Neural networks for Advanced modeling.", accepted for **J**ournal of **O**pen **S**ource **S**oftware.

N. Demo, M. Strazzullo, and G. Rozza (2023). "An extended physics informed neural network for preliminary analysis of parametric optimal control problems.", accepted for **C**omputers **A**nd **M**athematics **W**ith **A**pplications.

Artificial Intelligence: Optimal transport-inspired framework for DL in ROMs



Kernel POD maps

- Forward Map: Implicit feature space via kernel

$$F : \mathbb{R}^{N_h} \to \mathbb{R}^k;$$
$$\boldsymbol{u}_h \mapsto \boldsymbol{z} = \tilde{\boldsymbol{V}}^{\star T} g(\boldsymbol{u}_h),$$
$$g(\boldsymbol{u}_h) = [\kappa(\boldsymbol{u}_h, \boldsymbol{u}_h)]_{i=1}^{N_s} .$$

- Backward Map: Decoder of a CAE.

Wasserstein distance

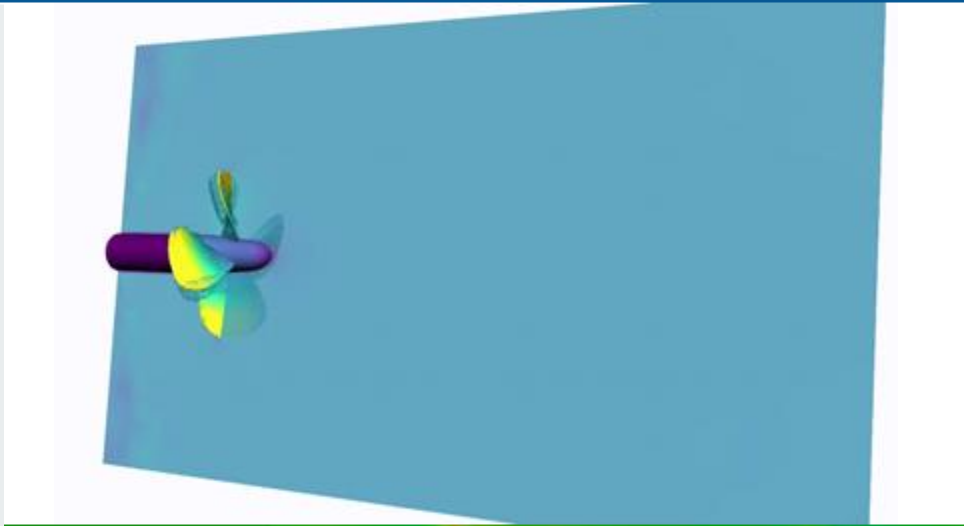
- Wasserstein based kernel;
- Neural Network training.

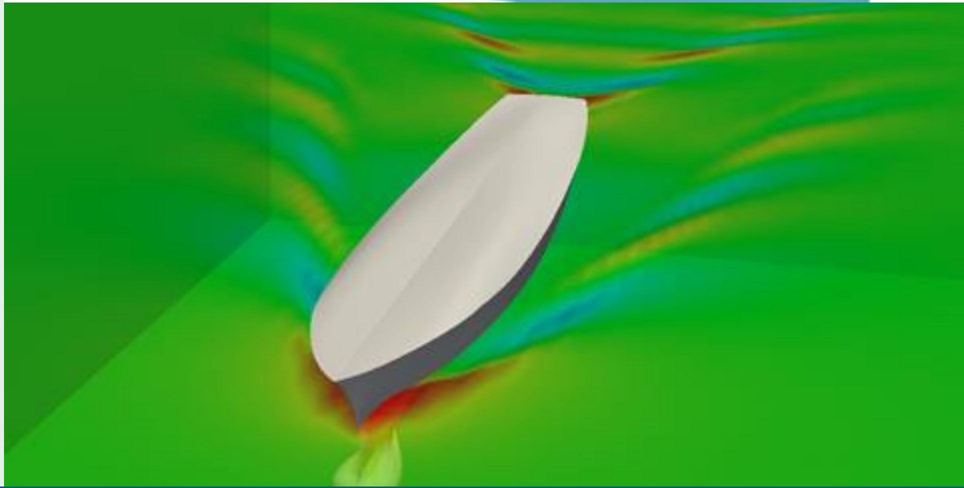
M. Khamlich, F. Pichi, & G. Rozza., (2023) Optimal Transport-inspired Deep Learning Framework for Slow-Decaying Problems: Exploiting Sinkhorn Loss and Wasserstein Kernel, *In preparation*.

Shape optimization in naval engineering

➔ Exploiting ROM in a shape optimization pipeline
➔ How to improve the efficiency in naval engineering applications?

Joint work with:
Anna Ivagnes, Nicola Demo



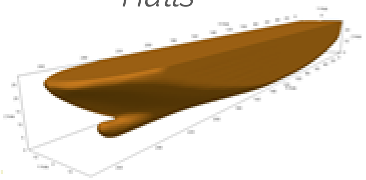


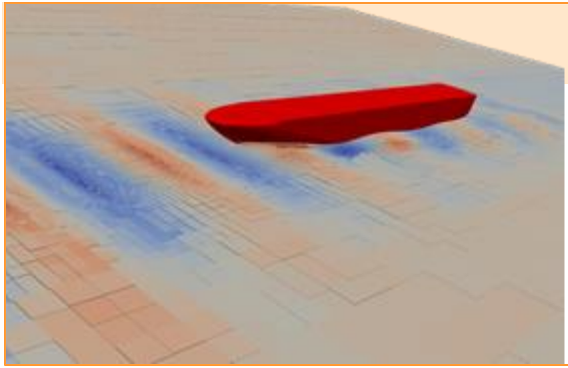
Motivation for naval design optimization

Goal:
optimize the design of a specific element of the ship to improve the performance

Propellers

Hulls





Optimization for different purposes

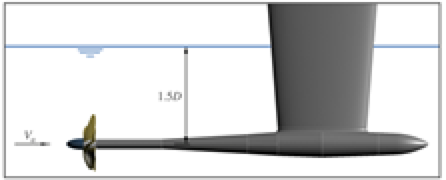
- Ensure comfort in yachts
- Avoid cavitation phenomena
- Increase efficiency
- Reduce vibrations

MICAD CETENA MCY engys FINCANTIERI

The propeller test case

The test case: open-water tests

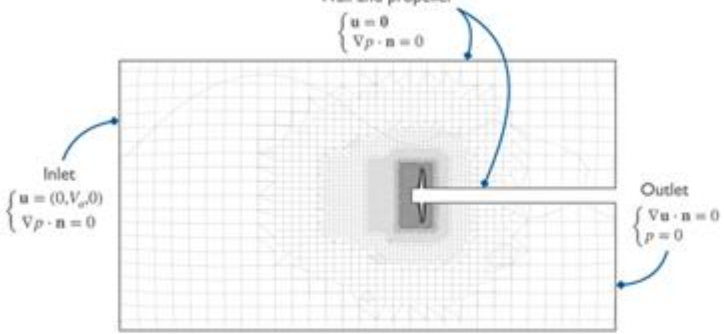
- Homogeneous inflow (velocity Va)
- Uniform and undisturbed flow conditions



The model: incompressible Navier-Stokes Equations

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} = -\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) + \nabla \cdot \nu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \nabla p \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

- ***Finite-Volume*** discretization
- ***RANS*** approach
- Turbulence model: κ-ω SST
- Mesh rotation: **Moving Reference Frame (MRF)**



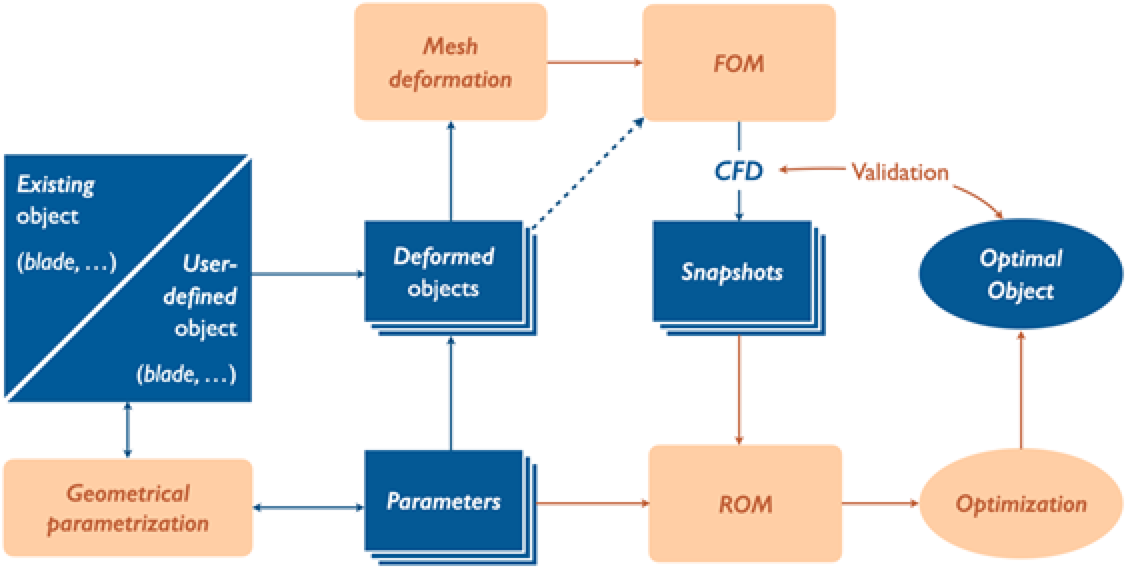
A slice of the mesh

Every simulation takes **24-48 hours** on our cluster in parallel on 55 cores

Unfeasible for optimization

A shape optimization pipeline using ROMs

A full pipeline exploiting **non-intrusive reduced order models**

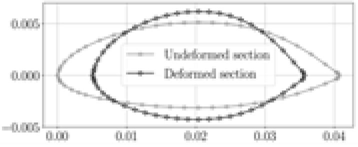


Ivagnes, Anna, Nicola Demo, and Gianluigi Rozza (2024). "A shape optimization pipeline for marine propellers by means of reduced order modeling techniques." International Journal for Numerical Methods in Engineering 125.7.

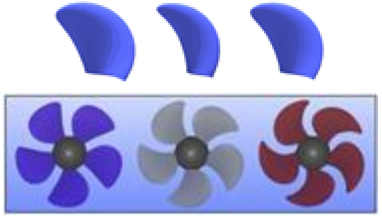
Geometric parametrization: two alternatives

Deformation through ***geometrical features*** (used for propellers)

- Select ***geometrical features*** (chord length, rake, thickness, ...)
- ***Deform the blades*** by modifying the parameters



Example of section deformation

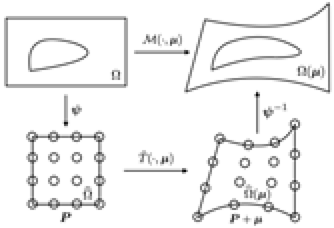


Example of blade/propeller deformation

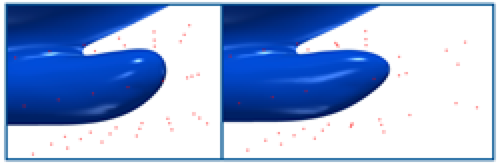
BladeX

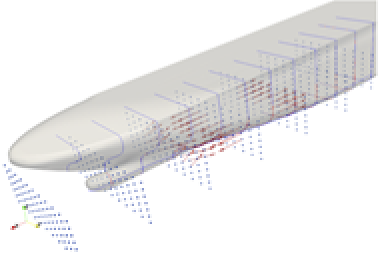
Library used

Deformation through ***Free Form Deformation*** (used for hulls)



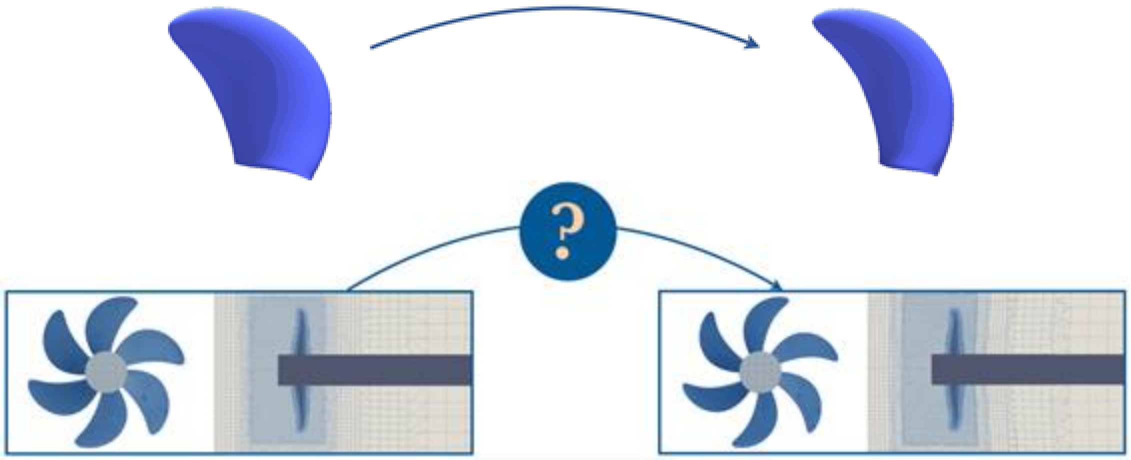
Strategy:
enclose the object in a cube, deform the cube, then back-map





Mesh deformation

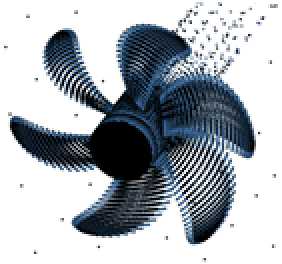
Problem: deform the mesh ***preserving the number of degrees of freedom*** in all simulations

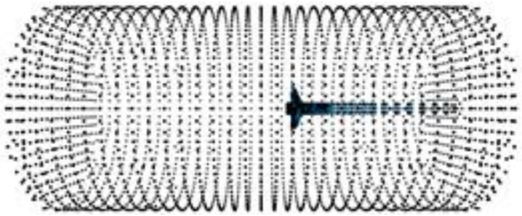


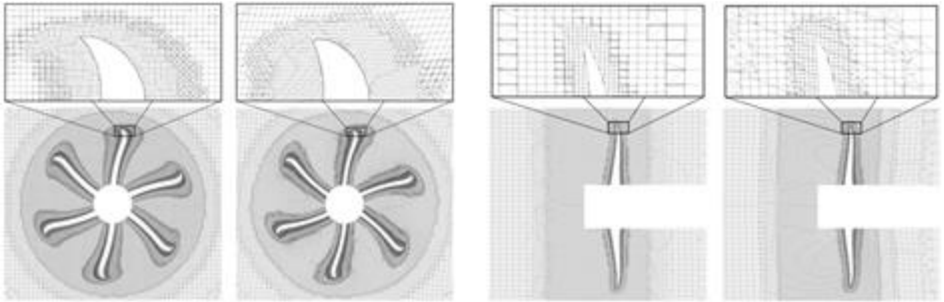
Mesh deformation

Solution: ***RBF interpolation technique***, using as ***control points*** the ***boundaries***

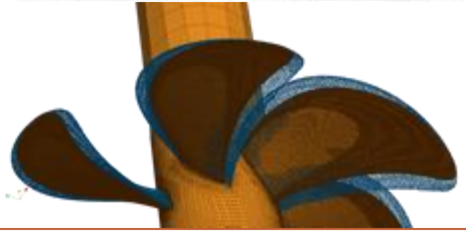
A look at the undeformed and deformed control points: blades (right), all boundaries (below).







Different deformed mesh slices (above); an example of mesh deformation on the propeller surface (right).



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Non-intrusive ROM performance

Two alternative ROM approaches in optimization

Standard ROM

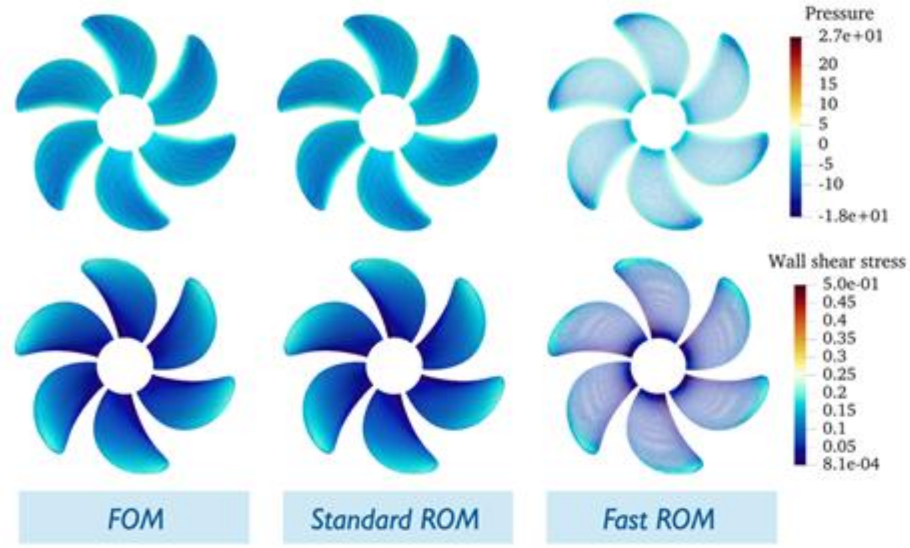
- fields evaluated at ***all blades points***
- needs to ***deform all blades points*** to compute the efficiency

5-6 minutes for each efficiency evaluation
Speed-up: ~ $\mathbf{10^2}$

Fast ROM

- fields evaluated at ***quadrature points***
- efficiency computed via ***quadrature formulas***

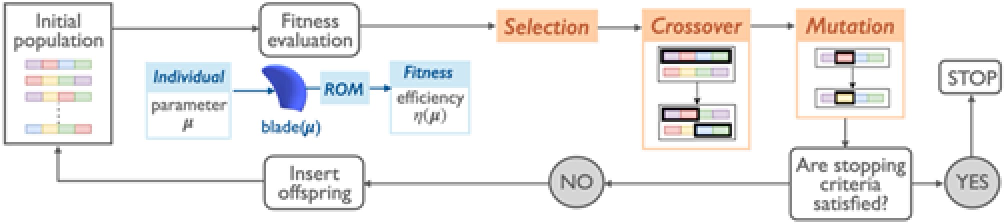
10-15 seconds for each efficiency evaluation
Speed-up: ~ $\mathbf{10^5}$



Ivagnes, Anna, Nicola Demo, and Gianluigi Rozza (2024). "A shape optimization pipeline for marine propellers by means of reduced order modeling techniques." International Journal for Numerical Methods in Engineering 125.7.

Optimization algorithm: results

The genetic algorithm: an evolution-inspired algorithm



Why genetic?

- Not stuck in *local minima*
- Not influenced on *initial guess*
- *Many* fitness evaluations

	Standard ROM	*Fast ROM*
Unconstrained optimization	+5.13 %	+3.24 %
Constrained optimization (physical/geometrical constraints)	+0.81 %	+0.80 %

Optimal blades (standard ROM)   *Optimal blades (fast ROM)*

Ivagnes, Anna, Nicola Demo, and Gianluigi Rozza (2024). "A shape optimization pipeline for marine propellers by means of reduced order modeling techniques." International Journal for Numerical Methods in Engineering 125.7.

Model Reduction Methods in CFD: state of the art and perspectives

Gianluigi Rozza

MathLab, Mathematics Area, SISSA International School for Advanced Studies, Trieste, Italy

Model Reduction and Machine Learning

CNRS RTTE
6 November 24

Intrusive Reduced Order Methods in a nutshell

- $()^{\mathcal{N}}$: "truth" full order method (FEM, FV, FD, SEM) – to be accelerated
- $()_N$: reduced order method (ROM) – *the accelerator*

* Input parameters:

$$\boldsymbol{\mu} \text{ (geometry, physical properties, etc.)}$$

* Parametrized PDE:

$$\mathcal{A}(u(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \rightsquigarrow \quad \underbrace{\boldsymbol{A}^{\mathcal{N}}(\boldsymbol{\mu})\boldsymbol{u}^{\mathcal{N}}(\boldsymbol{\mu}) = 0}_{\text{full order}} \quad \rightsquigarrow \quad \underbrace{\boldsymbol{A}_N(\boldsymbol{\mu})\boldsymbol{u}_N(\boldsymbol{\mu}) = 0}_{\text{reduced order}}$$

* Output:

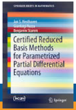
$$s(\boldsymbol{\mu}) \quad \approx \quad \underbrace{s^{\mathcal{N}}(\boldsymbol{\mu})}_{\text{full order}} \quad \approx \quad \underbrace{s_N(\boldsymbol{\mu})}_{\text{reduced order}}$$

* Input-Output evaluation:

$$\boldsymbol{\mu} \quad \to \quad s^{\mathcal{N}}(\boldsymbol{\mu}) \quad \to \quad s_N(\boldsymbol{\mu})$$

- **Reduced Basis Method(RB)**: continuation method in non-linear structural mechanics...
- **Proper Orthogonal Decomposition(POD)**: transient and turbulent flows...
- **Other methodologies**: Proper Generalized Decomposition (PGD), Hierarchical Model Reduction (HiMod).

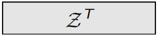
J. S. Hesthaven, G. Rozza, B. Stamm. *Certified Reduced Basis Methods for Parametrized Partial Differential Equations.* SpringerBriefs in Mathematics. Springer, 2015



Intrusive Reduced Order Methods in a nutshell

- $()^{\mathcal{N}}$: "truth" full order method (FEM, FV, FD, SEM) – to be accelerated
- $()_N$: reduced order method (ROM) – *the accelerator*

- **Offline**: very expensive preprocessing (full order): basis calculation (done *once*) after suitable parameters sampling (greedy, POD, ...)

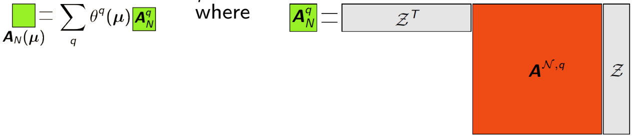


- **Online**: extremely fast (reduced order): real-time input-output evaluation

$$\boldsymbol{\mu} \rightarrow s_N(\boldsymbol{\mu})$$

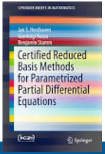
thanks to an efficient assembly of problem operators

$$\boldsymbol{A}_N(\boldsymbol{\mu}) = \sum_q \theta^q(\boldsymbol{\mu})\boldsymbol{A}_N^q, \text{ where } \boldsymbol{A}_N^q = \mathcal{Z}^T\boldsymbol{A}^{\mathcal{N},q}\mathcal{Z}$$



- Numerical issues: approximation stability, error bounds and stability factors, efficient (geometrical) parametrization, sampling, coupling, nonlinearities...

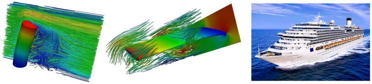
... reduction in parameter space

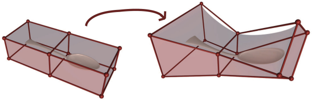


J. S. Hesthaven, G. Rozza, B. Stamm. *Certified Reduced Basis Methods for Parametrized Partial Differential Equations*. SpringerBriefs in Mathematics. Springer, 2015

Overview on the topics: from intrusive to non-intrusive ROM

- ROMs exploit a parametrized formulation of the problem. In particular, an efficient **geometrical parametrization** is required when interested in the variation of the domain/interface, such as in **shape optimization or fluid-structure interaction problems** $\Omega_o(\boldsymbol{\mu}) = \boldsymbol{T}(\Omega; \boldsymbol{\mu})$.
- **Focus: show some state of the art and perspectives in parametric flow problems treated in the reduced order context** for fluids
  - inverse problems;
  - shape optimization;
  - and some perspectives and challenges.





Shape parameterization for ROM

- Free-Form Deformations (FFD) [Lassila, Rozza, CMAME, 2010], [Salmoiraghi *et al.*, AMSES, 2016].
- Radial Basis Functions (RBF) [Manzoni *et al.*, IJNMBE, 2011].
- Transfinite Mapping (TM) [Løvgren, Maday, Rønquist, 2006], [Iapichino *et al.*, CMAME, 2012].
- Vascular shape parametrization [Ballarin *et al.*, JCP, 2016].
- Reduced inverse Distance Weighting [D'Amario et al, 2017].

Overview: our current efforts, aims and perspectives

- Towards **Real-Time** Computing and Visualization, through an **Offline–Online** computational paradigm that combines

High Performance Computing to **Advanced Reduced Order Modelling techniques**.

Offline:
HPC facilities, time demanding

"Science" driven

Online:
In situ, tablets or smartphones, real time

"Industrial needs" driven

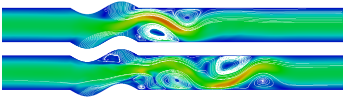
- **Export numerical simulations and scientific computing** in fields and places where at the state of the art there is still little exploitation.
- Development of new open-source tools based on reduced order methods:
  - **ITHACA**, **I**n real **T**ime **H**ighly **A**dvanced **C**omputational **A**pplications, as an add-on to integrate already well established CSE/CFD open-source software libraries (FV, SEM) with ROMs (OpenFoam, Nektar, FEniCS, Libmesh)
  - **RBniCS** as educational initiative (FEM) for newcomer ROM users (training).
  - **Argos** Advanced Reduced order modellinG Online **computational web server** for parametric Systems
  - **ATLAS**

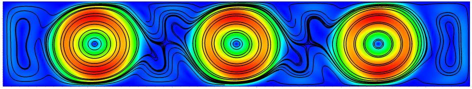
ITHACA | ITHACA - FV | ITHACA-SEM | ITHACA-DG | RBniCS | multiphenics | ARGOS | ATLAS

http://mathlab.sissa.it/cse-software

#CFD #intrusive #ROM
#supremizer # SUPG # VMS #inf-sup

ROM and stability
for fluid mechanics problems
with Francesco Ballarin, Giovanni Stabile, Shafqat Ali, Enrique Delgado





Reduced-order numerical simulations by POD-Galerkin ROM

- parametrized formulation of Navier-Stokes equations (modelling Newtonian fluid);
- offline stage:
  - intensive phase, on HPC architectures, to be done once;
  - Finite Element approximation of the problem for few values of the parameters (snapshots):

for $\boldsymbol{\mu} \in \mathcal{D}$, find $(\underline{\mathbf{u}}^{\mathcal{N}}(\boldsymbol{\mu}), \underline{\mathbf{p}}^{\mathcal{N}}(\boldsymbol{\mu})) \in \mathbb{R}^{\mathcal{N}_{\mathbf{u}}} \times \mathbb{R}^{\mathcal{N}_p}$,

large $\mathcal{N}$

$$\begin{bmatrix} A^{\mathcal{N}}(\boldsymbol{\mu}) + C^{\mathcal{N}}(\underline{\mathbf{u}}^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) & B^{\mathcal{N}}(\boldsymbol{\mu})^T \\ B^{\mathcal{N}}(\boldsymbol{\mu}) & O \end{bmatrix} \begin{bmatrix} \underline{\mathbf{u}}^{\mathcal{N}}(\boldsymbol{\mu}) \\ \underline{\mathbf{p}}^{\mathcal{N}}(\boldsymbol{\mu}) \end{bmatrix} = \begin{bmatrix} \underline{f}^{\mathcal{N}}(\boldsymbol{\mu}) \\ \underline{\mathbf{0}} \end{bmatrix}$$

  - [POD] Proper Orthogonal Decomposition (based on singular value decomposition) to extract optimal basis functions from the set of numerical simulations (snapshots) of the system to build $\mathcal{Z}$. [RB] Greedy as an alternative.

    Aubry et al. J. Fluid Mech. 1988; Ravindran, Int. J. Numer. Meth. Fluids, 2000
  - online stage

Reduced-order numerical simulations by POD-Galerkin ROM

- parametrized formulation of Navier-Stokes equations (modelling Newtonian fluid);
- offline stage:
  - intensive phase, on HPC architectures, to be done once;
  - Finite Element approximation of the problem for few values of the parameters (snapshots)
  - [POD] Proper Orthogonal Decomposition (based on singular value decomposition) to extract optimal basis functions from the set of numerical simulations (snapshots) of the system to build $\mathcal{Z}$.

    Build the correlation matrices $\mathbf{C}^{\boldsymbol{u}}, \mathbf{C}^{\boldsymbol{p}} \in \mathbb{R}^{N_{train} \times N_{train}}$, where N_{train} is the dimension of the training set and

    $$\mathbf{C}_{ij}^{\boldsymbol{u}} = (\underline{\boldsymbol{u}}^{\mathcal{N}}(\boldsymbol{\mu}_i), \underline{\boldsymbol{u}}^{\mathcal{N}}(\boldsymbol{\mu}_j)) \text{ and } \mathbf{C}_{ij}^{\boldsymbol{p}} = (\underline{\boldsymbol{p}}^{\mathcal{N}}(\boldsymbol{\mu}_i), \underline{\boldsymbol{p}}^{\mathcal{N}}(\boldsymbol{\mu}_j)) \qquad i, j = 1, \dots, N_{train}.$$

    Then we find $(\lambda_i^{\boldsymbol{u}}, v_i^{\boldsymbol{u}})$ and $(\lambda_i^{\boldsymbol{p}}, v_i^{\boldsymbol{p}})$ such that $\mathbf{C}^{\boldsymbol{u}} v_i^{\boldsymbol{u}} = \lambda_i^{\boldsymbol{u}} v_i^{\boldsymbol{u}}$ and $\mathbf{C}^{\boldsymbol{p}} v_i^{\boldsymbol{p}} = \lambda_i^{\boldsymbol{p}} v_i^{\boldsymbol{p}}$. We retain only the first $N_{\boldsymbol{u}}$ and $N_{\boldsymbol{p}}$ eigenvalues for pressure and velocity, respectively.
    The reduced space is $\text{span}\{\Phi_1^{\boldsymbol{u}}, \dots, \Phi_{N_{\boldsymbol{u}}}^{\boldsymbol{u}}, \Phi_1^{\boldsymbol{p}}, \dots, \Phi_{N_{\boldsymbol{p}}}^{\boldsymbol{p}}\}$, where the basis function $\Phi_i^{\boldsymbol{u}}$ and $\Phi_i^{\boldsymbol{p}}$ are the eigenvectors of $\lambda_i^{\boldsymbol{u}}$ and $\lambda_i^{\boldsymbol{p}}$, respectively.
    Aubry et al. J. Fluid Mech. 1988; Ravindran, Int. J. Numer. Meth. Fluids. 2000
  - online stage

Reduced-order numerical simulations by POD-Galerkin ROM

- parametrized formulation of Navier-Stokes equations (modelling Newtonian fluid);
- offline stage
- online stage:
  - inexpensive and very fast, on a laptop, to be done multiple times (for each new value of the parameters);
  - Galerkin projection over a reduced basis space:

for $\boldsymbol{\mu} \in \mathcal{D}$, find $(\underline{\mathbf{u}}_{\mathbf{N}}(\boldsymbol{\mu}), \underline{\mathbf{p}}_{\mathbf{N}}(\boldsymbol{\mu})) \in \mathbb{R}^{N_{\mathbf{u}}} \times \mathbb{R}^{N_p}$, $\boxed{N = N_{\mathbf{u}} + N_p \ll \mathcal{N}}$

$$\begin{bmatrix} A_{\mathbf{N}}(\boldsymbol{\mu}) + C_{\mathbf{N}}(\underline{\mathbf{u}}_{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) & B_{\mathbf{N}}(\boldsymbol{\mu})^T \\ B_{\mathbf{N}}(\boldsymbol{\mu}) & O \end{bmatrix} \begin{bmatrix} \underline{\mathbf{u}}_{\mathbf{N}}(\boldsymbol{\mu}) \\ \underline{\mathbf{p}}_{\mathbf{N}}(\boldsymbol{\mu}) \end{bmatrix} = \begin{bmatrix} \underline{f}_{\mathbf{N}}(\boldsymbol{\mu}) \\ \underline{\mathbf{0}} \end{bmatrix}$$

Inf-sup stabilization and pressure recovery

- inf-sup condition is **not** necessarily preserved by Galerkin projection in the online phase.
- reduced velocity space **enrichment** by supremizer solutions,

$$V_N = POD(\{\boldsymbol{u}^{\mathcal{N}}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{train}}; N_{\mathbf{u}}) \quad \oplus \quad POD(\{S^{\boldsymbol{\mu}^i} p^{\mathcal{N}}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{train}}; N_{\mathbf{s}}),$$
$$Q_N = POD(\{p^{\mathcal{N}}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{train}}; N_p),$$

where $S^{\boldsymbol{\mu}} : Q^{\mathcal{N}} \to V^{\mathcal{N}}$ is the **supremizer operator** given by

$$(S^{\boldsymbol{\mu}} p^{\mathcal{N}}, \boldsymbol{w}^{\mathcal{N}})_V = b(p^{\mathcal{N}}, \boldsymbol{w}^{\mathcal{N}}; \boldsymbol{\mu}), \quad \forall \boldsymbol{w} \in V^{\mathcal{N}}.$$

where $b(\cdot, \cdot; \boldsymbol{\mu}) = \int_\Omega p \mathrm{div} \boldsymbol{w} d\Omega$ (pressure-divergence term)

In order to fulfill an ***inf-sup condition at the reduced-order level*** too:

$$\beta_N(\boldsymbol{\mu}) = \inf_{\underline{\mathbf{q}}_N \neq \underline{\mathbf{0}}} \sup_{\underline{\mathbf{v}}_N \neq \underline{\mathbf{0}}} \frac{\underline{\mathbf{q}}_N^T B_N(\boldsymbol{\mu}) \underline{\mathbf{v}}_N}{\|\underline{\mathbf{v}}_N\|_{V_N} \|\underline{\mathbf{q}}_N\|_{Q_N}} \geq \tilde{\beta}_N > 0 \qquad \forall \boldsymbol{\mu} \in \mathcal{D}.$$

where $B_N(\boldsymbol{\mu})$ is the reduced-order matrix associated to the divergence term. ***(Rozza, Veroy. CMAME, 2007, Rozza et al, Numerische Mathematik, 2013. Ballarin et al. IJNME, 2015)***. Other options: residual-based stabilization procedures for POD-Galerkin ***(Caiazzo, Iliescu et al. JCP, 2014)***, Petrov-Galerkin ***(Dahmen; Carlberg; Abdulle, Budac)***, div-free approach ***(Lovgren et al.)***.

Inf-sup stabilization and pressure recovery

- inf-sup condition is **not** necessarily preserved by Galerkin projection in the online phase.
- reduced velocity space **enrichment** by supremizer solutions,

$$V_N = POD(\{\boldsymbol{u}^{\mathcal{N}}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{train}}; N_{\mathbf{u}}) \quad \oplus \quad POD(\{S^{\boldsymbol{\mu}^i} p^{\mathcal{N}}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{train}}; N_{\mathbf{s}}),$$
$$Q_N = POD(\{p^{\mathcal{N}}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{train}}; N_p),$$

where $S^{\boldsymbol{\mu}} : Q^{\mathcal{N}} \to V^{\mathcal{N}}$ is the **supremizer operator** given by

$$(S^{\boldsymbol{\mu}} p^{\mathcal{N}}, \boldsymbol{w}^{\mathcal{N}})_V = b(p^{\mathcal{N}}, \boldsymbol{w}^{\mathcal{N}}; \boldsymbol{\mu}), \quad \forall \boldsymbol{w} \in V^{\mathcal{N}}.$$

where $b(\cdot,\cdot;\boldsymbol{\mu}) = \int_\Omega p \mathrm{div} \boldsymbol{w} \, d\Omega$ (pressure-divergence term)

In order to fulfill an ***inf-sup condition at the reduced-order level*** too:

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Some ROM challenges in CFD: to higher Reynolds parametrized flows

- ROMs of parametrized viscous flows for low and moderate Reynolds number are well developed: we need to **increase Reynolds number** for several industrial applications.

- Offline–Online **stabilization techniques** for parametrized flows (geometry, physics) is derived from streamline upwind Petrov-Galerkin (SUPG), . . .

$$\sup_{\boldsymbol{v}_N \neq 0} \frac{b(\boldsymbol{v}_N, q_N; \boldsymbol{\mu})}{\|\boldsymbol{v}_N\|_{V_N}} + s(q_N, q_N)^{\frac{1}{2}} \geq \tilde{\beta}_N \|q_N\|_{Q_N} > 0, \quad \forall q_N \in Q_N, \forall \boldsymbol{\mu} \in \mathcal{D} \quad \text{(Generalized inf-sup).}$$

- A ROM **variational multiscale** approach in parametrized context towards turbulence modelling and a Smagorinski turbulent model have been recently proposed

  G. Stabile, F. Ballarin, G. Zuccarino and G. Rozza. A reduced order variational multiscale approach for turbulent flows, Advances in Computational Mathematics, 2019.

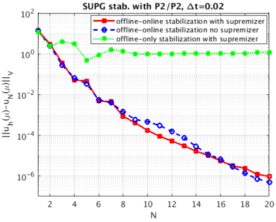
  F. Ballarin, T. Chacón Rebollo, E. Delgado Ávila, M. Gómez Mármol, and G. Rozza, *Certified Reduced Basis VMS-Smagorinsky model for natural convection flow in a cavity with variable height.* CAMWA, 2020. http://arxiv.org/abs/1902.05729

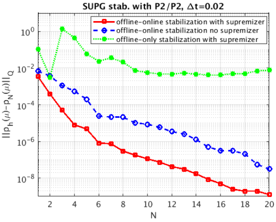
  T. Chacón Rebollo, E. Delgado Ávila, M. Gómez Mármol, F. Ballarin, and G. Rozza *On a certified Smagorinsky reduced basis turbulence model.* SIAM Journal on Numerical Analysis, 55 (2017) pp. 3047-3067

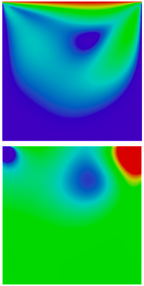
- Important expectations and needs dealing with **industrial and cardiovascular flows**.
- ROM developments in FV and also higher order methods.

Unsteady incompressible Navier-Stokes equations

- Numerical simulations on a lid driven cavity using FE discretization $\mathbb{P}_2/\mathbb{P}_2$.
- Classical **stabilization** technique is implemented in the high order and then projected on reduced basis.
- **RB stabilization** is based on Streamline Upwind Petrov Galerkin (SUPG) and compared with the supremizer enrichment approach
- A significant reduction in the computational cost of **offline-online stabilization** without supremizer could be achieved





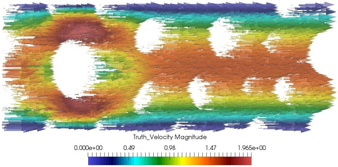


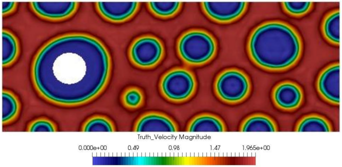
Error comparison for Velocity (left) and Pressure (right). Parameter range in offline stage is $Re \in [100, 200]$, FE dimension $\mathcal{N}$=3327, RB dimension, $N = 60$ (with supremizer), $N = 40$ (without supremizer).

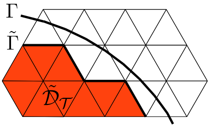
S. Ali, S. Hijazi, G. Stabile, F. Ballarin, G. Rozza, The effort of increasing Reynolds number in POD-Galerkin Reduced Order Methods: from laminar to turbulent flows, Numerical Methods for flows, Springer LNCSE, 2019.

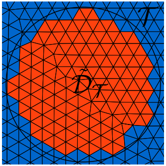
#Fluid Dynamics #Embedded-Immersed FEMs #ROMS on a Background Geometry

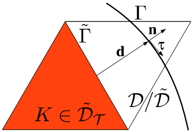
with Efthymios Karatzas, Francesco Ballarin, Giovanni Stabile, Guglielmo Scovazzi, Leo Nouveau, Nabil Atallah





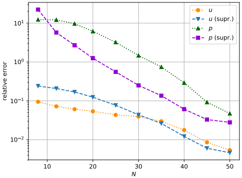


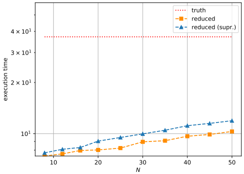


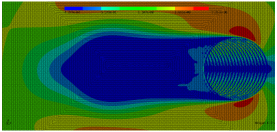


ROMS for systems with Parametric Geometry and Embedded FEMs

- **Equations:** **Multiphase fluid dynamics, viscous steady and unsteady incompressible flows,** Stokes, Navier-Stokes, Cahn-Hilliard
- **Methodology:** SBM, CutFEM, EBM/IBM, differences/**advantages** with respect to a **reference domain approach**





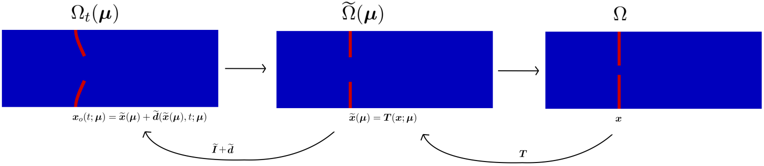


Supremizers enrichment:	No		Yes	
Number of modes	relative error u	relative error p	relative error u	relative error p
8	0.0947158	12.309881	0.2406999	22.319781
12	0.0723268	12.133591	0.2078557	5.7159319
16	0.0610052	9.6652163	0.1692787	2.6962056
20	0.0538906	6.1692750	0.1243368	1.2535779
30	0.0396132	1.4693532	0.0437348	0.2504069
40	0.0177170	0.2918072	0.0121903	0.0611154
50	0.0053882	0.0473412	0.0046300	0.0279857

E.N. Karatzas, G. Stabile, L. Nouveau, G. Scovazzi, G. Rozza. *A reduced basis approach for PDEs on parametrized geometries based on the shifted boundary finite element method and application to a Stokes flow*, CMAME, (347), pp. 568-587, 2019
E.N. Karatzas, F. Ballarin, G. Rozza, Projection-based reduced order models for a cut finite element method in parametrized domains, CAMWA, 2019

#FSI # TransportMap #convection-dominated

Monolithic ROMs for FSI problems with Francesco Ballarin, Monica Nonino and Yvon Maday



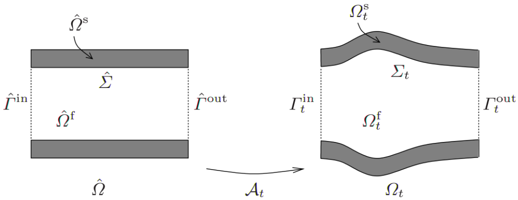
Formulation of FSI problems

- Fluid variables: $(\boldsymbol{u}_f, p, \boldsymbol{d}_f)$,
- Structure variables: $(\boldsymbol{u}_s, \boldsymbol{d}_s)$,
- Fluid-structure interaction problem three-fields formulation:

$$\begin{cases} F(\boldsymbol{u}_f, p, \boldsymbol{d}_f; \boldsymbol{d}_s) = 0, & \text{Fluid} \\ S(\boldsymbol{u}_s, \boldsymbol{d}_s) = 0, & \text{Structure} \\ I(\boldsymbol{d}_f, \boldsymbol{d}_s) = 0, & \text{Interface} \end{cases}$$

subject to interface (coupling) conditions

$$\begin{cases} \boldsymbol{d}_s - \boldsymbol{d}_f = 0 & \text{on } \Gamma, & \text{geometric continuity} \\ \boldsymbol{u}_s - \boldsymbol{u}_f = 0 & \text{on } \Gamma, & \text{velocity continuity} \\ \sigma_f \cdot n_f + \sigma_s \cdot n_s = 0 & \text{on } \Gamma, & \text{balance of normal forces.} \end{cases}$$



Reduced order monolithic formulation of FSI problems

Truth Finite Element discretization (P2-P1 Taylor-Hood)

For $\boldsymbol{\mu} \in \mathcal{D}$, solve large $\mathcal{N}$

$$F^{\mathcal{N}}(\boldsymbol{u}_f^{\mathcal{N}}(\boldsymbol{\mu}), p^{\mathcal{N}}(\boldsymbol{\mu}), \boldsymbol{d}_f^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{d}_s^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \text{Fluid}$$

$$S^{\mathcal{N}}(\boldsymbol{u}_s^{\mathcal{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \text{Structure}$$

$$I^{\mathcal{N}}(\boldsymbol{d}_f^{\mathcal{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \text{Interface, coupled conditions}$$

OFFLINE – Space construction and matrices assembling

- Space construction by **Proper Orthogonal Decomposition** for **global** variables.
- Additional computations related to inf-sup stabilization procedure by means of supremizer enrichment $\rightarrow$ accurate pressure recovery for balance of normal forces. [Ballarin et al., 2015], [Rozza *et al.*, 2012], [Rozza, Veroy, 2007].

ONLINE – Galerkin projection over the enriched space

For $\boldsymbol{\mu} \in \mathcal{D}$, solve $\mathbf{N} \ll \mathcal{N}$

$$F^{\mathbf{N}}(\boldsymbol{u}_f^{\mathbf{N}}(\boldsymbol{\mu}), p^{\mathbf{N}}(\boldsymbol{\mu}), \boldsymbol{d}_f^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{d}_s^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \textbf{Reduced} \text{ fluid}$$

$$S^{\mathbf{N}}(\boldsymbol{u}_s^{\mathbf{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \textbf{Reduced} \text{ structure}$$

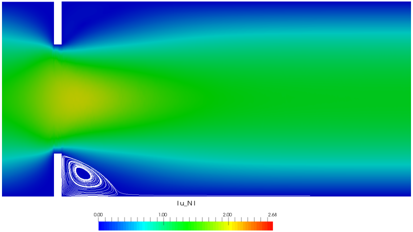
$$I^{\mathbf{N}}(\boldsymbol{d}_f^{\mathbf{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0 \quad \textbf{Reduced} \text{ interface, coupled conditions}$$

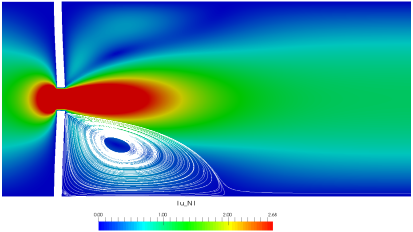
Our approach:

- POD–Galerkin method for **global** variables $\boldsymbol{u}, p, \boldsymbol{d}$ (monolithic approach), time dependent,
- capability to parametrize the initial configuration (geometry).

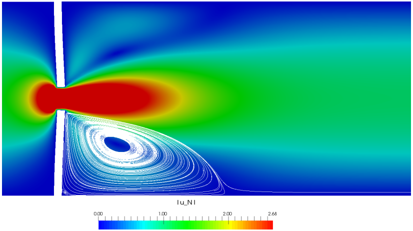
Ongoing applications to cardiovascular modelling

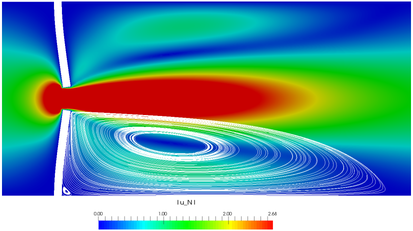
Increase leaflet length: *(same inlet velocity)*





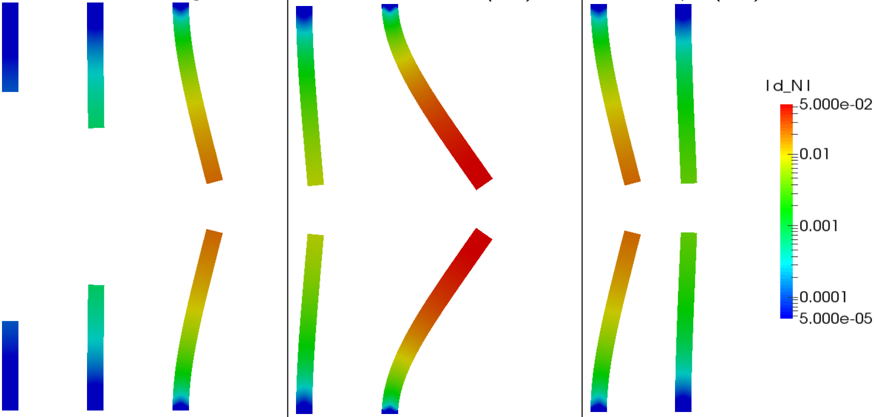
Increase inlet velocity: *(same leaflet length)*





Ongoing applications to cardiovascular modelling

Increase leaflet length: | *Increase inlet vel. (5×):* | *Increase μ_s (8×):*



(same inlet velocity, same material properties) | *(same leaflet length, same material properties)* | *(same leaflet length, same inlet velocity)*

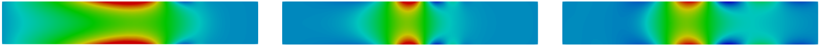
- *Ballarin, Rozza. POD–Galerkin monolithic reduced order models for parametrized fluid-structure interaction problems. IJNMF, 82(12):1010–1034, 2016.*
- *F. Ballarin, G. Rozza, Y. Maday. Reduced-order semi-implicit schemes for fluid-structure interaction problems. MS&A, vol. 17, 2017. Springer [segregated approach]*

Reduction of Kolmogorov n-width for FSI

- Time dependent and coupled problem: tube with a fluid, and solid walls at the top and at the bottom. The problem is transport dominated.

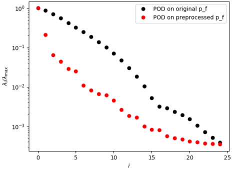
Example: pressure wave($t = 0.0024, 0.006, 0.011$) travelling in the domain, causing a slow decay of the Kolmogorov n-width of the solution manifold:

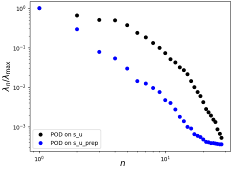
Offline step (preprocessing): stretch the snapshots so that we move the peak of the pressure wave at the same point. Example below ($t = 0.0024, 0.006, 0.011$):

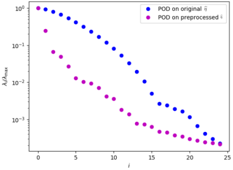


N. Cagniart, Y. Maday, B. Stamm. Model Order Reduction for problems with large convection effects. https://hal.upmc.fr/hal-01395571. 2016.

Results: comparison of the rate of decay of the singular values of the POD on the pressure, on the fluid velocity supremizer and on the displacement.



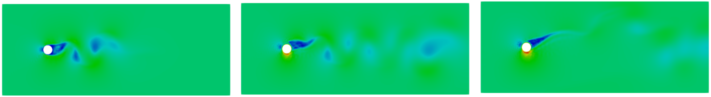




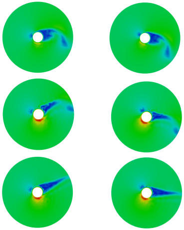
A CFD test case: flow past a rotating cylinder

- Time dependent problem; fluid past a cylinder rotating counterclockwise.

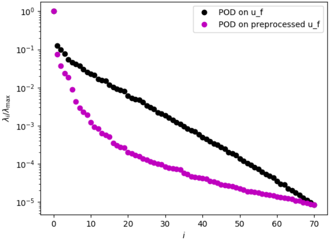
Example: fluid velocity $\mathbf{u}_f$ behaviour. The direction of propagation of the vortex changes due to the rotation of the cylinder.



Preprocessing: rotate the snapshots back so that the direction of propagation of the vortex is horizontal. Below: example and comparison in the POD.



Before (left) and after (right) the preprocessing.

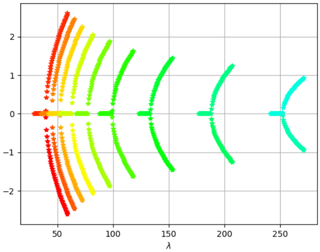


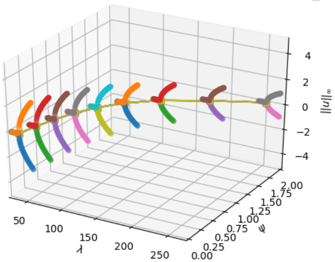
☺ Improvement in the rate of decay of more than one order of magnitude!

M. Nonino et al. Overcoming slowly decaying Kolmogorov n-width by transport maps: application to model order reduction of fluid dynamics and fluid–structure interaction problems. https://arxiv.org/abs/1911.06598. 2019.

#Advanced #CFD & #Structural #Mechanics

ROM for Stability and Bifurcations Studies
with Martin Hess, Federico Pichi
Annalisa Quaini, Max Gunzburger and Anthony Patera

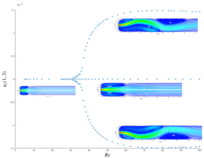


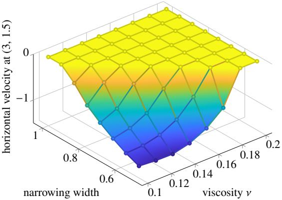


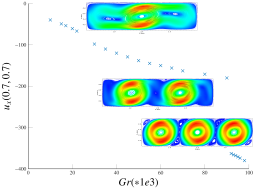
Bifurcation analysis with ROMs in fluid dynamics

Bifurcation and stability analysis of parametrized Navier-Stokes models by global and localized ROMs

- **Stability studies** in nonlinear problems are very expensive.
- Understand and detect complex phenomena, such as **bifurcations**, leading to loss of uniqueness with changing geometry and physical parameters, using spectral element simulations.
- Efficient reduced numerical techniques to detect **steady and Hopf bifurcations and branching**.
- continuation, eigenvalues analysis, long-term goal: use in multi-physics studies.







– M. Hess, A. Quaini, G. Rozza. "Reduced Basis Model Order Reduction for Navier-Stokes equations in domains with walls of varying curvature", IJCFD 2019, ArXiv arxiv.org/abs/1901.03708

– M. Hess, A. Quaini, and G. Rozza, "A Spectral Element Reduced Basis Method for Navier-Stokes Equations with Geometric Variations", 2018, Enumath Proc.ArXiv arxiv.org/abs/1812.11051

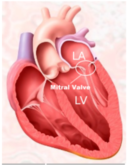
– M. Hess, A. Alla, A. Quaini, G. Rozza, and M. Gunzburger, "A Localized Reduced-Order Modeling Approach for PDEs with Bifurcating Solutions", CMAME 2019, ArXiv arxiv.org/abs/1807.08851

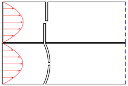
– F. Pichi, G. Rozza, Reduced basis approaches for parametrized bifurcation problems held by non-linear Von *Kármán* equations, JSC, 2019.

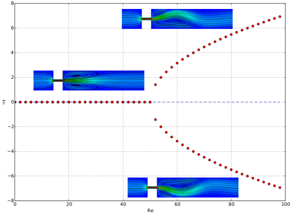
– M. Pintore, F. Pichi, M. Hess, G. Rozza, C. Canuto, Efficient computation of bifurcation dagrams with a deflated approach to reduced basis spectral element method, ACOM, 2020.

Some ROM challenges in CFD

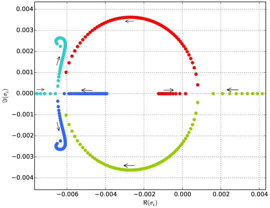
- **Complex CFD problems** in 3D setting characterized by bifurcations, e.g. Coanda effect during **mitral valves** regurgitation, influence of more complex geometries and multiphysics on bifurcations and stability.

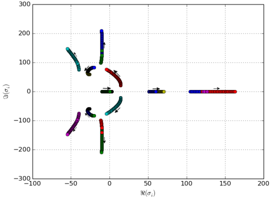






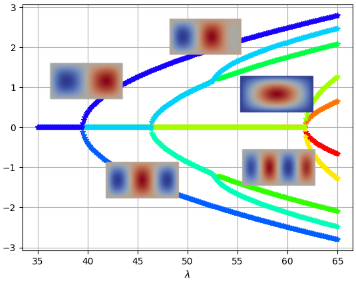
Investigations on bifurcations and loss of uniqueness of the solution require ROM for parametrized eigenvalue analysis. [Pitton, Rozza, 2017, Journal of Scientific Computing; Pitton, Quaini, Rozza, 2017, Journal of Computational physics]

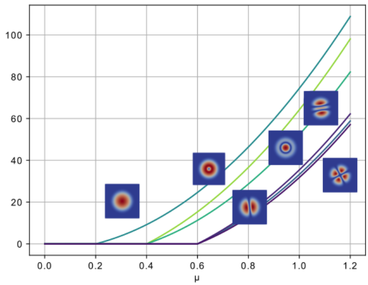




Some ROM challenges in Structural Mechanics

- **Computational mechanics problems** to study the deformation of a plate under compression (load λ and shapeψ) and the bifurcations of the Von Kaŕmań model through the linearized eigenproblem. [Pichi, F. , Rozza, G., 2019, Reduced basis approaches for parametrized bifurcation problems held by non-linear Von *Kármán* equations, J. Scie. Comp.]



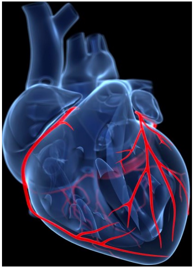


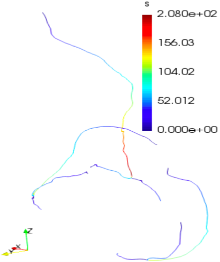
- Secondary bifurcations, better computations of parametric stability factors
- **Quantum mechanics problems** to study the Gross–Pitaevskii equation that describes the ground state of a quantum system of identical bosons.
  [Pichi, F. , Quaini, A., Rozza, G, 2020, Reduced deflation technique in bifurcating phenomena: application to the Gross–Pitaevskii equation, SIAM SISC]

Further investigations on: Empirical Interpolation techniques, Neo-Hookean beam 2D/3D problem and a posteriori error estimate are in progress.
FVG - MIT project ROM2S

#Applications
ROMs # CFD # OFCPs # CAD # CABGs

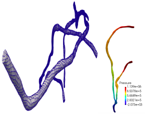
Parametrized reduced order optimal control for blood flows in patients' specific geometries
with Zakia Zainib, Francesco Ballarin
Piero Triverio, Laura Jiménez, Stephen Fremes





Mysteries of the heart: U of T Engineering professor developing solutions for coronary artery disease with mathematical models

Professor Piero Triverio (ECE) at centre, and collaborators Drs. Stephen Fremes (right), Laura Jiménez-Juan (left) of Sunnybrook Health Sciences Centre and Professor Gianluigi Rozza of SISSA are developing a study that could provide surgeons with better information about coronary artery disease (Credit: Jessica MacInnis)



Triple Coronary Artery Bypass Grafts (CABGs)

- Medical image data (CT-scan) from **Sunnybrook Health Sciences Center, Toronto, Canada**.
- Three grafts attached to three different diseased arteries,
  - Right internal mammary artery (RIMA) to left anterior descending artery (LAD).

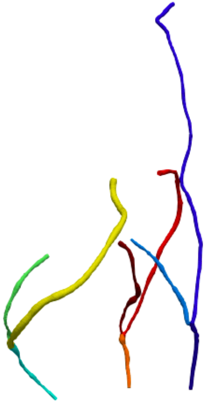
    RIMA LAD

  - Vein graft to first obtuse marginal artery (OM1).

    Vein graft OM1

  - Vein graft to posterior descending artery (PDA).

    Vein graft PDA



F. Auricchio, M. Conti, A. Lefieux, S. Morganti, A. Reali, G. Rozza, and A. Veneziani. Cardiovascular Mechanics, chapter: **Computational Methods in Cardiovascular Mechanics. CRC Press Taylor and Francis Group, 2018.**

Physiological data assimilation

Problem description:

Navier-Stokes equations constrained **boundary control** with **physical parametrization**, and **geometrical and physiological data assimilation**.

$$\min_{(\boldsymbol{v},\boldsymbol{u})} \mathcal{J}\left(\boldsymbol{v}(\mu), p(\mu), \boldsymbol{u}(\mu)\right) = \frac{1}{2}\int_{\Omega} |\boldsymbol{v}(\mu) - \boldsymbol{v}_d|^2 + \frac{\alpha}{2}\int_{\Gamma_{out}} |\boldsymbol{u}(\mu)|^2$$

$$\text{subject to} \begin{cases} -\eta\Delta\boldsymbol{v}(\mu) + (\boldsymbol{v}(\mu)\cdot\nabla)\boldsymbol{v}(\mu) + \nabla p(\mu) = \boldsymbol{0}, & \text{in } \Omega \\ \nabla\cdot\boldsymbol{v}(\mu) = 0, & \text{in } \Omega \\ \boldsymbol{v}(\mu) = \boldsymbol{v}_{in}, & \text{on } \Gamma_{in} \\ \boldsymbol{v}(\mu) = \boldsymbol{0}, & \text{on } \Gamma_{wall} \\ \eta\nabla\boldsymbol{v}(\mu)\cdot\boldsymbol{n} - p(\mu)\boldsymbol{n} = \boldsymbol{u}(\mu) & \text{on } \Gamma_{out} \end{cases}$$

- Patient-specific computational domain Ω.
- Patient-specific physiological data $\boldsymbol{v}_d$ acquired through 4D-MRI.

The goal: rely on simplier Neumann boundary conditions, but tune $\boldsymbol{u}(\mu)$ to best match $\boldsymbol{v}_d$ acquired by measurement of the velocity profile.

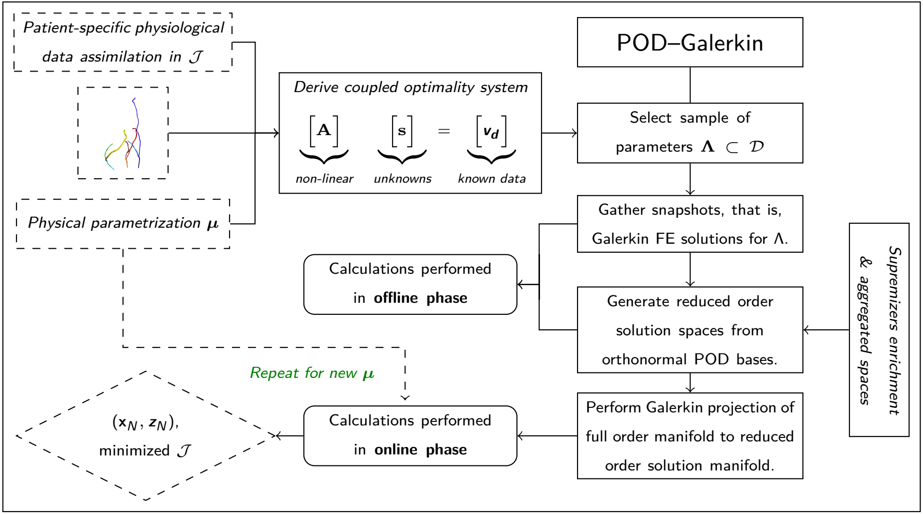


Figure: Reduced order optimal control pipeline: an overview

Negri, Manzoni, and Rozza, Comp. Math. App., 2015.

Negri, Rozza, Manzoni, and Quarteroni, SIAM J. Sci. Comp., 2013.

Reliability of the reduced order model

Test case: Vein graft to OM1, $\boldsymbol{\mu} = \mathrm{Re} \in [45, 50]$

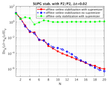


Figure: Velocity magnitude

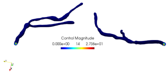


Figure: Control magnitude

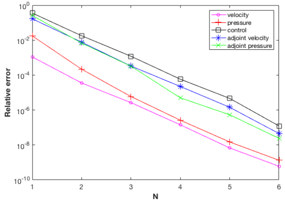


Figure: Relative error b/w FE and POD approximations of variables

	FE approx.	ROM approx.
Mesh size	27398	-
Degrees of freedom	280274	43
CPU time (secs)	634	118 (online)

Table: Computational performance

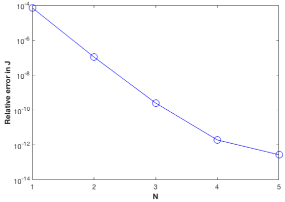
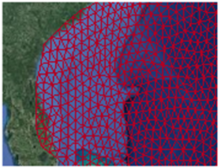
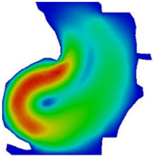


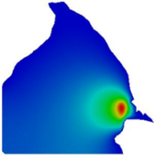
Figure: Relative error b/w FE and POD reduction in $\mathcal{J}$

Zainib et al., *in preparation*, 2019.

#Applications #Environmental #CFD #DataAssimilation #InverseProblems

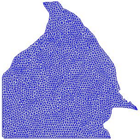
Reduced Order Methods for Parametrized Optimal Flow Control in Environmental Marine Sciences with Maria Strazzullo and Francesco Ballarin

Pollutant Control on Gulf of Trieste, Italy

Motivations: forecasting, data assimilation, ecological and touristic and geographical interest.
Collaborations: National Institute of Oceanography and Applied Geophysics, OGS, Trieste, Italy.
Problem formulation
$y \in H^1_{\Gamma_D}(\Omega), u \in \mathbb{R}, y_d \in \mathbb{R}$ (safeguard threshold)



Weak formulation

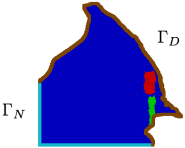
Minimise with respect to
$(y(\boldsymbol{\mu}), u(\boldsymbol{\mu})) \in Y \times U$

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

constrained to an advection-diffusion state equation:

$$a(y(\boldsymbol{\mu}), q) = c(u(\boldsymbol{\mu}), q), \qquad \forall q \in Q.$$

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).



Weak Formulation of the Parametric Inverse problem

- $a : Y \times Q \to \mathbb{R}$:

$$a(y, q, \boldsymbol{\mu}) = \int_{\Omega} (\nu(\boldsymbol{\mu}) \nabla y \cdot \nabla q + \boldsymbol{\beta}(\boldsymbol{\mu}) \cdot \nabla y q) \, d\Omega,$$

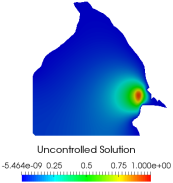
- $c : U \times Q \to \mathbb{R}$:

$$c(u, q) = Lu \int_{\Omega_u} q \, d\Omega_u, \quad [L = 10^3 \to \text{ non-dimensional system}]$$

Parameters ($\mathcal{D} = [0.5, 1] \times [-1, 1] \times [-1, 1]$)

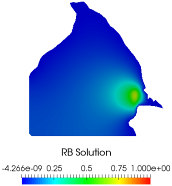
$\nu(\boldsymbol{\mu}) \equiv \mu_1$ is the diffusivity parameter,

$\boldsymbol{\beta}(\boldsymbol{\mu}) = [\beta_1(\mu_2), \beta_2(\mu_3)]$ is the transport field,



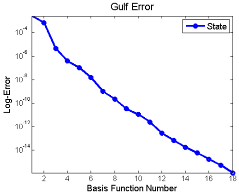
Control and cost functional value for several parameters

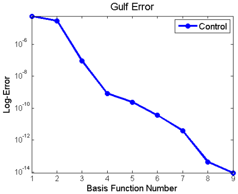
	$\boldsymbol{\mu}$	u	J_r
No wind	(1,0,0)	$7.6901 \cdot 10^{-1}$	$5.1320 \cdot 10^{-5}$
Bora	(1,-1,1)	$7.3698 \cdot 10^{-1}$	$4.9167 \cdot 10^{-5}$
Scirocco	(1,1,-1)	$8.0800 \cdot 10^{-1}$	$5.3417 \cdot 10^{-5}$

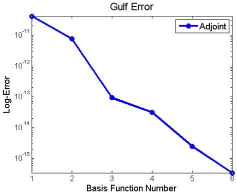


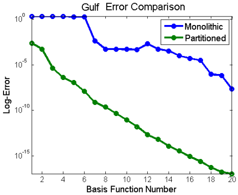
Time of a run: $t_{\mathcal{N}} = 2.79s, t_N = 2.41 \cdot 10^{-2}s$.
Dimensions: $\mathcal{N} = 5639$ and $N = 20$.

Numerical Results: FE – POD Errors









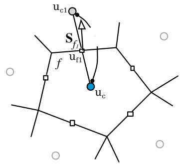
Parameter: $\boldsymbol{\mu} = (1, -1, 1)$.
Sampling distribution for POD: Uniform.
Training set dimension: 100.

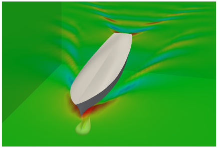
Bora Errors. *Bottom left*: monolithic (one POD for $U(\boldsymbol{\mu}) = (y(\boldsymbol{\mu}), u(\boldsymbol{\mu}), q(\boldsymbol{\mu}))$) and partitioned (different POD reductions for state, control and adjoint variables) error comparison.

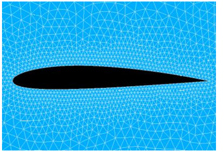
[Strazzullo et al., Model Reduction for Parametrized Optimal Control Problems in Environmental Marine Sciences and Engineering. SIAM SISC, 40:4, B1055-B1079, 2018]

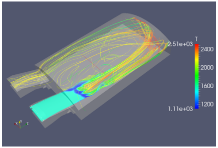
#Applications #Industrial #CFD

ROM for Finite Volume Approximations and Industrial Flows (Higher Reynolds Numbers) with Giovanni Stabile, Saddam Hijazi, Matteo Zancanaro and Michele Girfoglio









Overview of the physical problems of interest

- The interest is in **viscous steady and unsteady parametrized incompressible/compressible flows** with **moderate-high Reynolds number**
- Possible applications can be found in **naval** and **nautical** engineering, **aeronautical** engineering and **industrial** engineering.
- In general any application dealing with incompressible fluid dynamic problems that has the response depending on **parameter changes** (Reynolds Number, Grashof Number, Geometrical parameters ..)

Why Finite Volumes?

The finite element method is nowadays the standard in the reduced order modelling community so why to use a different discretisation technique?

☺ One can find well developed open source libraries, OpenFOAM is today probably the most spread CFD open-source solver.

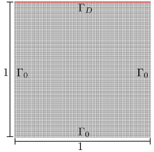
☺ For increasing Reynolds numbers there are less problems concerning stability and several turbulence models are already available.

G. Stabile, S. Hijazi, A. Mola, S. Lorenzi, and G. Rozza. *POD-Galerkin reduced order methods for CFD using finite volume discretization: vortex shedding around a circular cylinder*. Communications in Applied and Industrial Mathematics, 8(1), pp. 210-236, 2017.

Numerical examples

The lid driven cavity problem

The first proposed benchmark consists into the well known lid driven cavity problem:



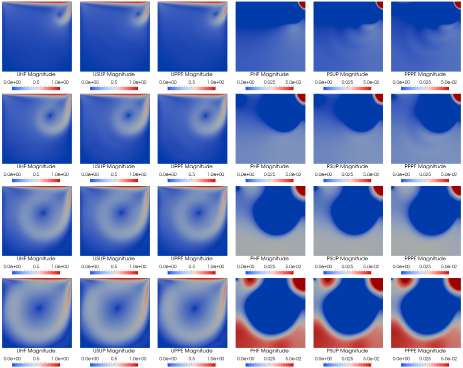
	Γ_D	Γ_0
$\boldsymbol{u}$	$\boldsymbol{u} = (1,0)$	$\boldsymbol{u} = (0,0)$
p	$\nabla p \cdot \boldsymbol{n} = 0$	$\nabla p \cdot \boldsymbol{n} = 0$

The mesh is structured and counts 40000 quadrilateral cells, 200 on each dimension of the square. The kinematic viscosity is equal to $\nu = 1 \times 10^{-4} \text{m}^2/\text{s}$ that leads to a Reynolds number of 10000.

In this case no parametrization is introduced.

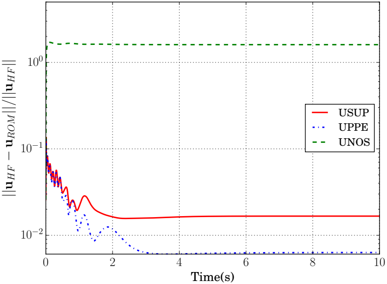
Comparison of the velocity and pressure fields for high fidelity, SUP-ROM and PPE-ROM.

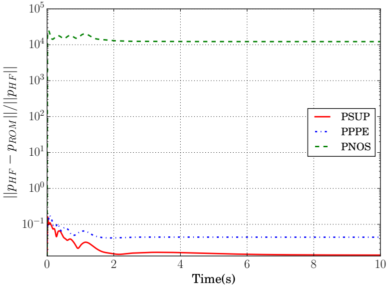
The fields are depicted for different time instant equal to $t = 0.2\text{s}, 0.5\text{s}, 1\text{s}$ and 5s.



Numerical examples

The L^2 norm of the relative error over time for three different models.

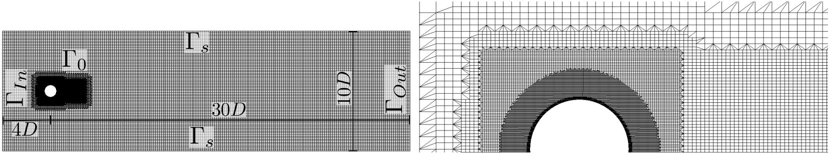




The table contains the cumulative eigenvalues for the lid driven cavity test. The last column contains the value of the inf-sup constant, in the supremizer stabilization case, for different different number of supremizer modes and with a fixed number of velocity and pressure modes.

N Modes	$\boldsymbol{u}$	p	$\boldsymbol{s}$	β
1	0.978946	0.975406	0.980260	9.264e-05
2	0.994184	0.991528	0.995232	9.264e-05
3	0.997737	0.995385	0.997912	7.175e-04
4	0.998990	0.998116	0.999400	7.175e-04
5	0.999483	0.999270	0.999844	7.175e-04
10	0.999971	0.999971	0.999997	1.551e-02

The flow around a circular cylinder

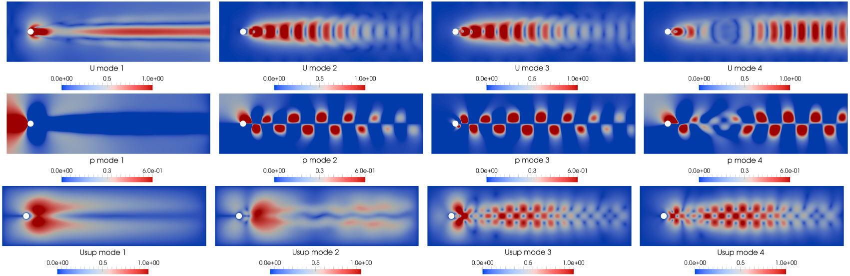


	Γ_{In}	Γ_0	Γ_s	Γ_{Out}
$\boldsymbol{u}$	$\boldsymbol{u} = (1,0)$	$\boldsymbol{u} = (0,0)$	$\boldsymbol{u} \cdot \boldsymbol{n} = 0$	$\nabla \boldsymbol{u} \cdot \boldsymbol{n} = 0$
p	$\nabla p \cdot \boldsymbol{n} = 0$	$\nabla p \cdot \boldsymbol{n} = 0$	$\nabla p \cdot \boldsymbol{n} = 0$	$p = 0$

The properties of the presented algorithms have been tested also with the benchmark of the **laminar flow around a circular cylinder**. In this case the viscosity have been parametrized and results refer to a parameter non experimented in the full order simulations. The parameter space is given by **5 different** values of the viscosity: $\nu \in [0.005, 0.01]$. These values of viscosity result into the values of the Reynolds number $\text{Re} \in [100, 200]$.

Numerical examples

First four modes for velocity pressure and supremizers

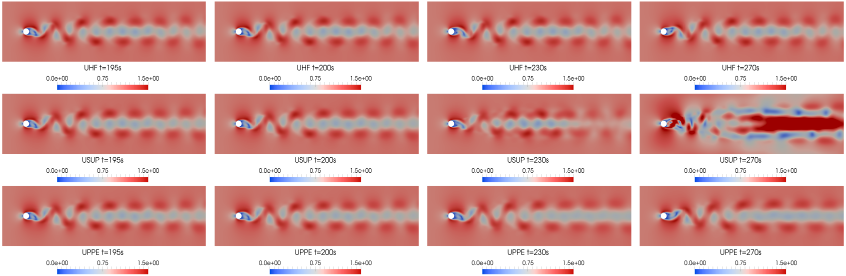


Cumulative eigenvalues

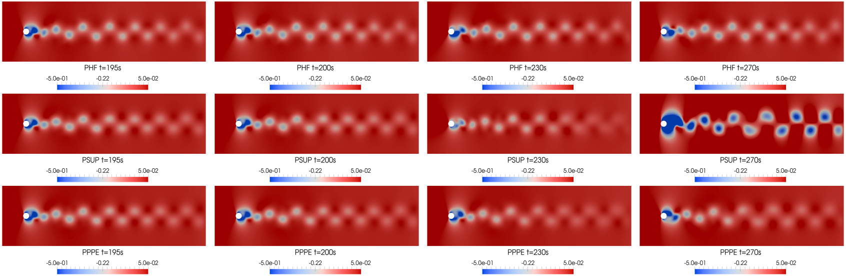
N Modes	$\boldsymbol{u}$	p	$\boldsymbol{s}$	β
1	0.390813	0.793239	0.921046	2.608e-04
2	0.598176	0.85809	0.941746	4.492e-04
3	0.802176	0.911636	0.961438	7.869e-03
4	0.879096	0.934997	0.978072	1.662e-02
5	0.949519	0.955578	0.98669	1.662e-02
10	0.986025	0.992347	0.998307	1.098e-01
15	0.995922	0.997994	0.999732	1.199e-01

Numerical examples

Comparison of the velocity field

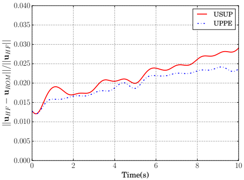


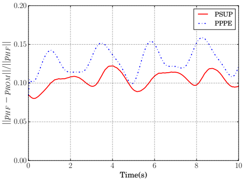
Comparison of the pressure field



Numerical examples

Comparison on the same time window ans computational costs





	Cavity Exp.	Cylinder Exp.
HF	25min	18.5min $\times$ 6proc.
SUP-ROM	7.64s	3.14s
PPE-ROM	4.86s	0.971s

- The **velocity** field is reproduced in a more accurate way using the **Poisson equation** approach. This is due to the "pollution" given by the non-necessary supremizer modes.
- On the other side the **pressure** field is better reproduced using a supremizer approach.
- The **cavity** example has run serially with OpenFOAM 5.0 (i7 laptop).
- The **cylinder** example has run in parallel with OpenFOAM 5.0.
- The reduced order models have run in serial in **ITHACA-FV**. It is available on github `https://github.com/mathLab/ITHACA-FV`.
- In the worst case the speed up is equal to approx. 200.

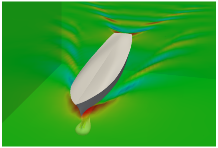
ITHACA - FV

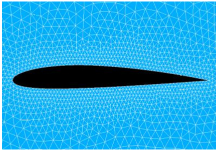
G. Stabile and G. Rozza, Stabilized Reduced order POD-Galerkin techniques for finite volume approximation of the parametrized Navier–Stokes equations, Computer & Fluids, 2018.

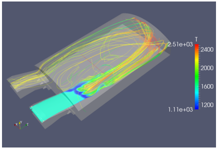
S. Ali, S. Hijazi, G. Stabile, F. Ballarin, G. Rozza, The effort of increasing Reynolds number in POD-Galerkin Reduced Order Methods: from laminar to turbulent flows, FEF. Springer LNCSE, 2019.

#CFD #turbulence #FV
#datadriven #ROM

ROM and Finite Volume Discretization
for fluid mechanics of turbulent flows
with Saddam Hijazi, Giovanni Stabile and Andrea Mola

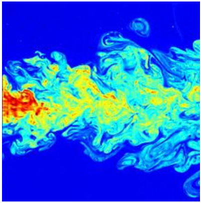


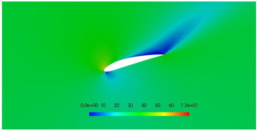


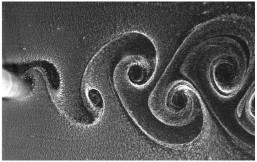


Reduced order methods for turbulent flows

- The goal is to develop reduced order methods dedicated for the treatment of **turbulent flows**.
- Development of Reduced Order Models which merge **projection-based** methods and **data-driven** techniques.
- The model has been tested on benchmark cases like the **Pitz-Daily** case and the flow around a **circular cylinder**.
- The **Reynolds** number in the cases is up to $\mathbf{Re} = 10^4\text{-}10^6$.







RANS Equations.

- The $k - \omega$ turbulence model, has been used in this work

$$
\begin{cases}
\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) = \text{lam. terms} + g(\nu_t) & \text{in } \Omega \times [0, T], \\
\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 & \text{in } \Omega \times [0, T], \\
\boldsymbol{u}(t, \boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\mu}) & \text{on } \Gamma_{In} \times [0, T], \\
\boldsymbol{u}(t, \boldsymbol{x}) = \boldsymbol{0} & \text{on } \Gamma_0 \times [0, T], \\
(\nu \boldsymbol{\nabla} \boldsymbol{u} - p\boldsymbol{I})\boldsymbol{n} = \boldsymbol{0} & \text{on } \Gamma_{Out} \times [0, T], \\
\boldsymbol{u}(0, \boldsymbol{x}) = \boldsymbol{k}(\boldsymbol{x}) & \text{in } (\Omega, 0), \\
\nu_t = F(k, \omega), & \text{in } \Omega, \\
\text{Transport-Diffusion equation for } k, & \\
\text{Transport-Diffusion equation for } \omega, &
\end{cases}
$$

k is the turbulent kinetic energy
ω is the rate of dissipation for turbulent kinetic energy

- One could project the standard Navier Stokes equations without the eddy viscosity contribution on the modes computed using a stabilized FOM but **this approach fails**. $\rightarrow$ We have to consider the contribution given by the additional eddy viscosity term.

The Reduced Order Model

- Classical projection approach consists of **decomposing all turbulence variables** then projecting the additional PDEs onto the spaces spanned by the POD modes of the turbulence variables, namely:

$$k(\boldsymbol{x}, t; \boldsymbol{\mu}) \approx \sum_{i=1}^{N_k} e_i(t, \boldsymbol{\mu}) \beta_i(\boldsymbol{x}) \quad , \quad \omega(\boldsymbol{x}, t; \boldsymbol{\mu}) \approx \sum_{i=1}^{N_\omega} f_i(t, \boldsymbol{\mu}) \gamma_i(\boldsymbol{x}).$$

- This approach is **problem dependent**, where a different ROM has to be developed for each turbulence model, which makes the approach inconvenient, instead another idea is to decompose just the **the eddy viscosity field**.

$$\nu_t(\boldsymbol{x}, t; \boldsymbol{\mu}) \approx \sum_{i=1}^{N_{\nu_t}} g_i(t, \boldsymbol{\mu}) \eta_i(\boldsymbol{x}).$$

- The projection of the momentum equation gives:

$$\begin{cases} \boldsymbol{M}\dot{\boldsymbol{a}} = \nu(\boldsymbol{B} + \boldsymbol{B_T})\boldsymbol{a} - \boldsymbol{a}^{\boldsymbol{T}}\boldsymbol{C}\boldsymbol{a} + \boldsymbol{g}^{\boldsymbol{T}}(\boldsymbol{C_{T1}} + \boldsymbol{C_{T2}})\boldsymbol{a} - \boldsymbol{H}\boldsymbol{b}, \\ \boldsymbol{P}\boldsymbol{a} = \boldsymbol{0}, \end{cases}$$

where $\boldsymbol{g}$ is the vector of the coefficients $[g_i(t, \boldsymbol{\mu})]_{i=1}^{N_{\nu_t}}$.

The Reduced Order Model

- The problem is now to **compute the coefficients g** of the eddy viscosity equations **without relying on the projection** of the equations $\rightarrow$ **POD-I**.
- The **proper orthogonal decomposition with interpolation** is a method to approximate the numerical solution of a parametric partial differential equation as combination of few solutions computed for some properly chosen parameters.

$$\forall \boldsymbol{\mu}_k \in \mathcal{P}_{train}, \quad \nu_t(\mu_k) \approx \nu_t^N(\boldsymbol{\mu}_k) = \sum_{i=1}^{N} g_i(\boldsymbol{\mu}_k)\eta_i,$$

$$\nu_t^N{}_{NEW} = \sum_{i=1}^{N} g_i(\boldsymbol{\mu}_{NEW})\eta_i.$$

- Each function $g_i(\mu)$ is approximated using **approximated interpolant functions.**
- It relies only on the **snapshots**: it does not require any information about the system (**non-intrusive** approach).
- The interpolation is carried out using **Radial Basis Functions.**

Steady state case: the backstep

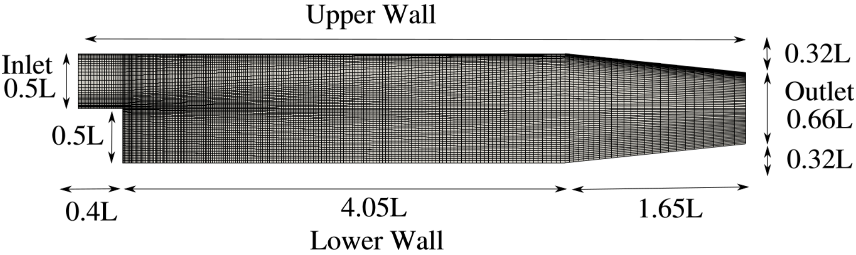


Figure: The computational domain used in the numerical simulations, L is equal to 50.8 meters.

The **parameter vector** is $\mu = [\mu_1, \mu_2]$
μ_1: the magnitude of the velocity at the inlet
μ_2: the inclination of the velocity with respect to the inlet which is measured in degrees.

Numerical results : Pitz-Daily benchmark steady case

Velocity results

- Fixed viscosity value $\nu = 10^{-3}$
- Parametrized inlet velocity in inclination and magnitude $\mu_1 \in [0.18, 0.3]$ and $\mu_2 \in [0, 30]$, **Reynolds** number ranges from 9.144×10^3–1.524×10^4

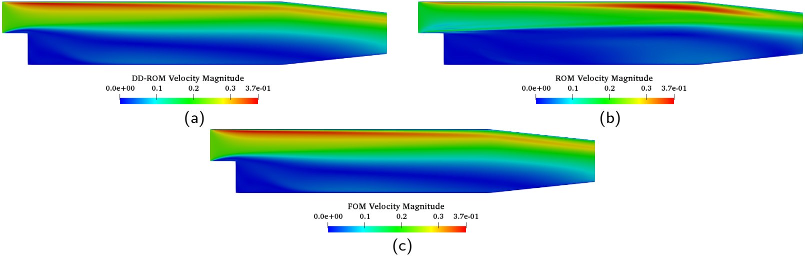
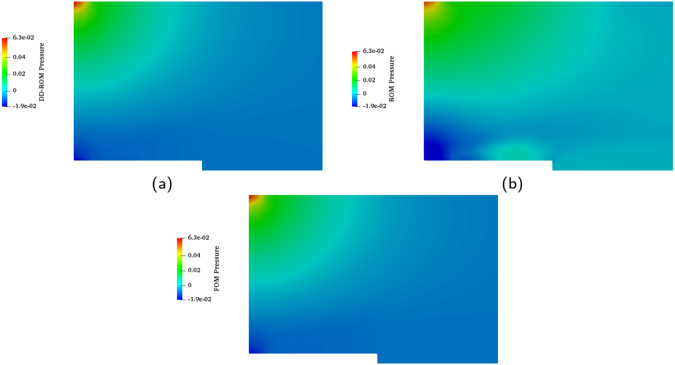


Figure: Velocity fields for $\boldsymbol{\mu}^* = (0.22089, 24.484)$: (a) shows the DD-ROM Velocity, while in (b) one can see the ROM Velocity (without viscosity incorporated in ROM), and finally in (c) we have the FOM Velocity.

S. Hijazi, S. Ali, G. Stabile, F. Ballarin, G. Rozza (2018) The Effort of Increasing Reynolds Number in Projection-Based Reduced Order Methods: from Laminar to Turbulent Flows, *FEF*. Springer LNCSE, 2019.

Pressure results

- The relative L^2 error are 2.957% and 222.96% for DD-ROM and ROM, respectively.



(a) (b) (c)

Figure: Pressure fields for $\boldsymbol{\mu}^* = (0.22089, 24.484)$: (a) shows the DD-ROM Pressure, while in (b) one can see the ROM Pressure (without viscosity incorporated in ROM), and finally in (c) we have the FOM Pressure.

Numerical results : Flow around a cylinder, unsteady case

- Results for the mixed **Data-Driven** and projection-based Reduced Order Model (DD-ROM) proved accuracy and efficiency compared to the ones obtained from a fully projection-based strategy.

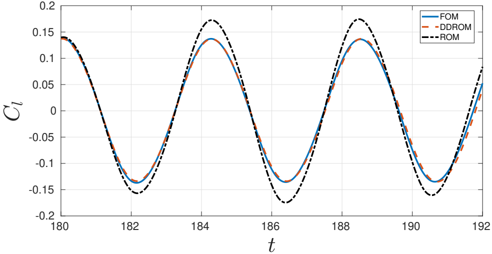


Figure: FOM,ROM and DD-ROM lift coefficients for the forces acting on the cylinder, in this case $Re = 10^4$.

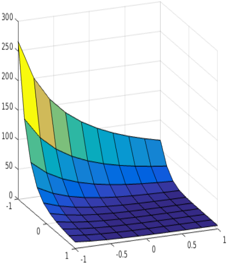
- DD-ROM relative error is in the range of $1 - 5$ %, while ROM has a relative error of 20%.
- $T_{CPU_{FOM}} = 525.32\ s$, $T_{CPU_{DD-ROM}} = 1.095\ s$
- Speed up of 479.

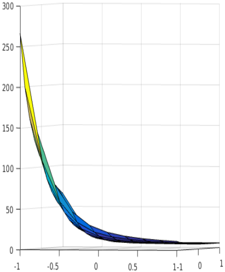
S. Hijazi, G. Stabile, A. Mola, G. Rozza. Data-Driven POD–Galerkin reduced order model for turbulent flows POD–Galerkin reduced order model for turbulent flows, *Submitted*, 2019.

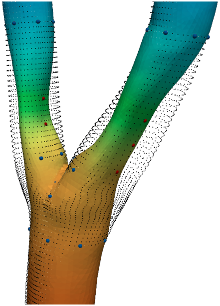
Shape parametrization # Active subspaces # POD-Galerkin # Carotid arteries

Combined parameter and model reduction with shape parametrization by active subspaces and POD-Galerkin

with Marco Tezzele







Active subspaces property

In many cases the dimension of the parametrised problem is only artificially high

- Active subspaces property identifies a set of important directions in the space of all inputs.

$$f : \mathbb{R}^m \to \mathbb{R} \qquad \mathbf{x} \in \mathbb{R}^m$$

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

$$\mathbf{C} = \mathbf{W} \boldsymbol{\Lambda} \mathbf{W}^T$$

f is a scalar function that takes as arguments the parameters x

C is the uncentered covariance matrix of the gradients of f, symmetric, positive semidefinite

E is the expected value and rho a probability density function

- We define the active subspace to be the range of the **first n eigenvectors** of W

$$\mathbf{W} = [\mathbf{W_1} \quad \mathbf{W_2}] \in \mathbb{M}^{m \times m} \qquad \boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda_1} & \\ & \boldsymbol{\Lambda_2} \end{bmatrix}$$

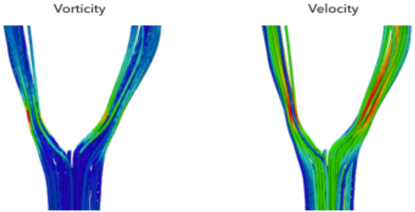
- With the basis identified, we can map forward to the active subspace. So **y is the active variable** and z the inactive one. The **surrogate model** g is used to approximate f

$$\mathbf{y} = \mathbf{W}_1^{\mathbf{T}} \mathbf{x} \in \mathbb{R}^n \qquad \mathbf{z} = \mathbf{W}_2^{\mathbf{T}} \mathbf{x} \in \mathbb{R}^{m-n} \qquad f(\mathbf{x}) \approx g(\mathbf{W}_1^{\mathbf{T}} \mathbf{x}) = g(\mathbf{y})$$

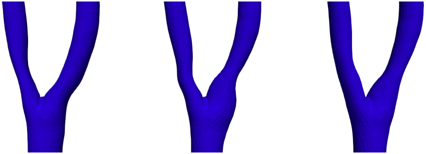
Constantine, Active subspaces: Emerging ideas for dimension reduction in parameter studies, SIAM, 2015.

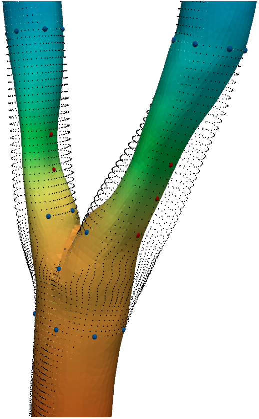
Flow across parametrised carotid bifurcations

- Vessels geometry strongly influences hemodynamics behaviour.
- The output function is the relative pressure drop of the two branches, computing the integral of the pressure on selected sections.



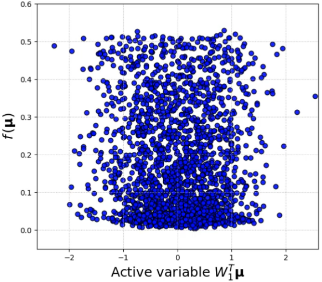
- We deform the carotid after the bifurcation moving 10 RBF control points (in red) solving an interpolation system.

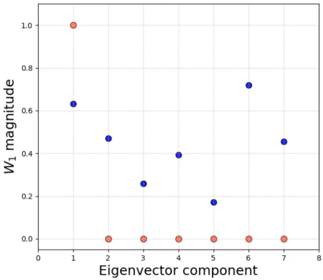




Deformed carotid with the deforming control points (red) and the undeformed state (black)

Active Subspaces - A quadratic example

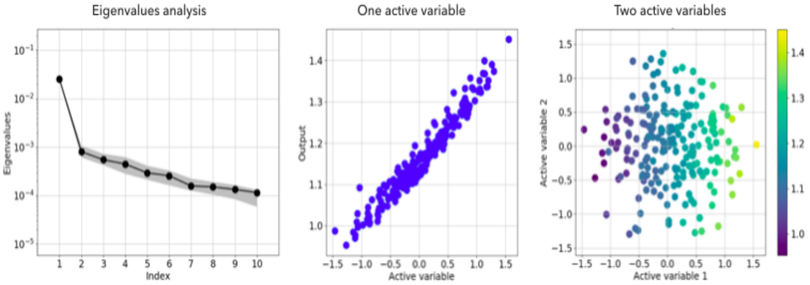




M. Tezzele, F. Ballarin and G. Rozza "Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD-Galerkin methods", *Mathematical and Numerical Modeling of the Cardiovascular System and Applications*, 2018.
M. Tezzele, F. Salmoiraghi, A. Mola, G. Rozza. "Dimension reduction in heterogeneous parametric spaces with application to naval engineering shape design problems", Advanced Modeling and Simulation in Engineering Sciences, 2018.

Spectral analysis

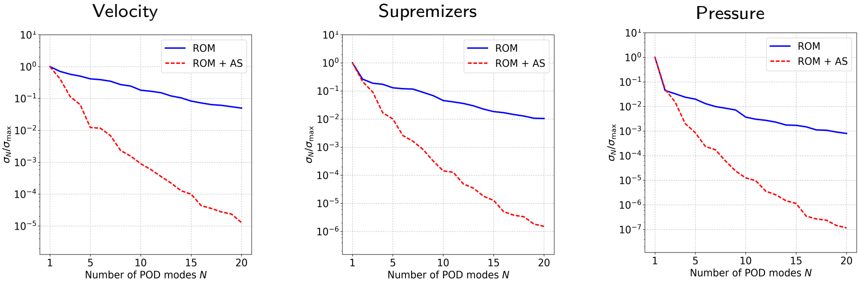
- The two dimensional active subspace spanned by the first two eigenvectors of the covariance matrix seems to better capture the behaviour of the output function. We use this information perform a further reduction by a POD-Galerkin ROM.
- We exploit a 2-dimensional active subspace to compute the POD snapshots in a reduced space with respect to the full 10-dimensional parameter space.
- Typical reduced space dimensions and computational speedup for cardiovascular flows: 500:1.



Tezzele, Ballarin, and Rozza, Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD-Galerkin methods. Contributed chapter SEMA/SIMAI 2018.

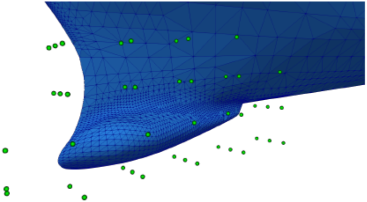
POD analysis

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



- The standard approach presents a slower decay, meaning that it has to deal with a considerably larger solution manifold.
- The combined methodology is able to reach relative errors which are up to one order of magnitude smaller when compared to the standard one, for both velocity and pressure when $N = 20$.

#GeometricalMorphing #Industrial #applications #FFD A full Monolithic data-driven ROMs computational for FSI problems pipeline with Marco Tezzele, Nicola Demo, Andrea Mola

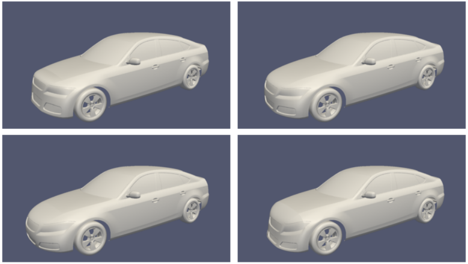


PyGeM: Python Geometrical Morphing

- PyGeM is a python library using Free Form Deformation, Inverse Distance Weighting, and Radial Basis Function interpolation technique to parametrize and morph complex geometries. It is developed by F. Salmoiraghi, N. Demo, and M. Tezzele

- The main focus of PyGeM is to interact with the major industrial file formats used for CAD management. Since it has to integrate itself in the industrial workflow we have chosen python

Morphing of the bumper using an OpenFOAM file. DrivAer model.



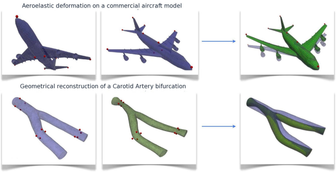
- It allows to handle:
  - Computer Aided Design files (.iges, .step and .stl)
  - Mesh files (.unv and OpenFOAM)
  - Output files (.vtk)

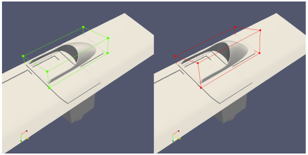
PyGeM on Github: github.com/mathLab/PyGeM

Efficient and accurate geometrical parametrization techniques

- At the state of the art free-form parametrization techniques for geometries are receiving a growing interest, in view of strong integration with CAD tools, as well as for design and shape optimization
- Extending isogeometric analysis (IGA) for viscous f ows in the reduced basis context

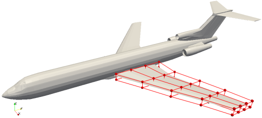
$$T(\underline{x}, \mu) : \Omega \to \Omega_0(\mu)$$

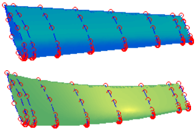




Underwater Blue Efficiency

MONTECARLOYACHTS





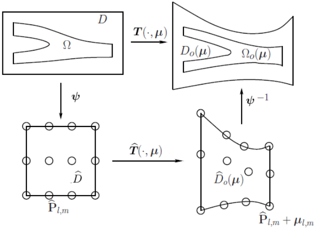
In collaboration with: F. Salmoiraghi, F. Ballarin, L. Heltai, A. Mola, M. Tezzele, N. Demo (SISSA), H. Telib, A. Scardigli (Optimad-PoliTo), D. Forti (EPFL)

Tool for the automatic shape parametrization

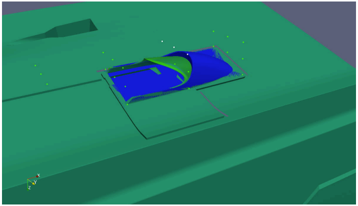
1. Mapping the physical domain to the reference one: ψ

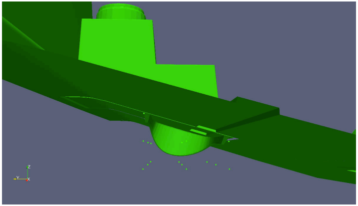
2. Moving some control points to deform the lattice: $\hat{T}$

3. Mapping back to the physical domain: ψ^{-1}



FFD: composition of the three maps $$T(\cdot,\mu) = (\psi^{-1} \circ \hat{T} \circ \psi)(\cdot,\mu)$$



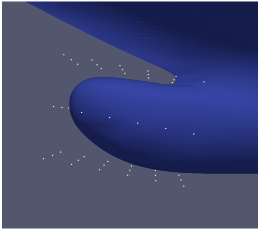


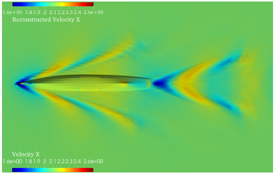
Reduced Order Model for industrial shape problems

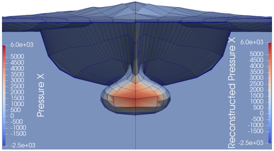
original hull → FFD → FV → DMD → PODI → OPT → optimized hull

In collaboration with Fincantieri, leader in cruise ship manifacturing, we developed an innovative pipeline involving **data-driven** reduced order modeling techniques for shape optimization in naval problems.

- **Shape parametrization** (FFD)
- **Proper orthogonal decomposition with interpolation**
- **Dynamic mode decomposition**







PyGeM EZyRB PyDMD

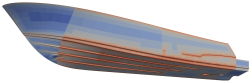
FINCANTIERI

REGIONE AUTONOMA FRIULI VENEZIA GIULIA

FSE FRIULI VENEZIA GIULIA POR 2014 2020

Reduced Order Model for industrial shape problems

- **POR FESR: SOPHYA** the main goal of the project is to **improve planing yacht** hulls the performance in **non-calm sea** conditions. A set of specific methodologies have been developed to be able to **parameterize the hull** geometry and carry out a **shape optimization** campaign based both on high fidelity **RANS** and non-intrusive **ROM** simulations.
- **POR FESR: PRELICA** the main goal of the project is to **improve ship propeller** performance both in terms of **thrust** and **acoustic emissions**. A specific python package (**BladeX**) has been developed to generate **parametrized propeller** geometries. The optimal propeller shape has been identified making use of both high order **LES** and non-intrusive **ROM** hydroacoustic simulations.



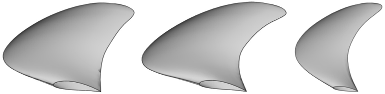
SOPHYA

POR FESR 2014 2020 Friuli Venezia Giulia

prelica

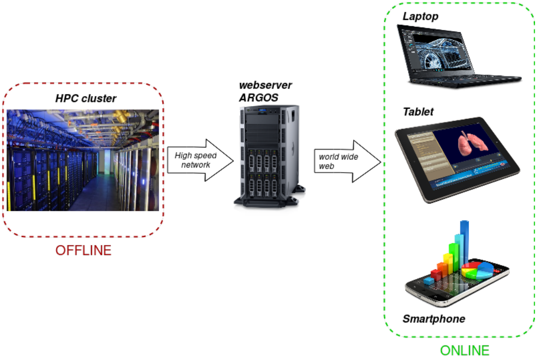
REGIONE AUTONOMA FRIULI VENEZIA GIULIA

BladeX



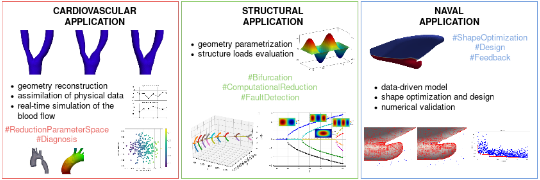
Vision and Perspective: to real-time computing

Model order reduction for web server: from biomedical to naval applications



CSE-Apps

- HPC, data science
- Web computing
- Digital twin
- 3D printing
- SMACT Industry4.0



Conclusion

- It is time to better integrate **Data, Modelling, Analysis, Numerics, Control, Optimization and Uncertainty Quantification** in a **new parametrized, reduced and coupled paradigm**.
- We need to draw the attention to the fact that **"Science and Industry advance with Mathematics"**.
- **Applied Mathematics as propeller for Innovation** and Technology Transfer by a new generation of computational scientists.

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Thanks for your attention!

Sponsors

- **European Research Council Executive Agency**, ERC CoG 2015 AROMA-CFD, GA 681447, 2016-2021.
- MIUR-PRIN project “Mathematical and numerical modelling of the cardiovascular system, and their clinical applications”, 2014-2016
- INDAM-GNCS 2015, “Computational Reduction Strategies for CFD and Fluid-Structure Interaction Problems”
- INDAM-GNCS 2016-2017 “Numerical methods for model order reduction of PDEs”
- COST, **European Union Cooperation in Science and Technology**, TD 1307 EU-MORNET Action (`http://www.eu-mor.net`)
- PAR-FSC 2014-2020, Regione Friuli Venezia Giulia, UBE
- POR-FESR, 2014-2020, Regione Friuli Venezia Giulia, SOPHYA, PRELICA, UBE 2
- TRIM, INSEAN-CNR, 2016
- HPC resources: CINECA, INFN, SISSA-ICTP
- MIUR FARE-X-AROMA-CFD project
- MIT projects: "Probabilistic Multi-disciplinary Ship Design using Reduced Order Methods and Machine Learning Tools", "ROM2S Reduced Order Methods at MIT and SISSA".

Thanks for your attention!