Surrogate Modelling by Reduced Order Methods and Scientific Machine Learning for Digital Twins

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SISSA

SISSA START-UP

FAST » COMPUTING

IMSI,
University of Chicago, US
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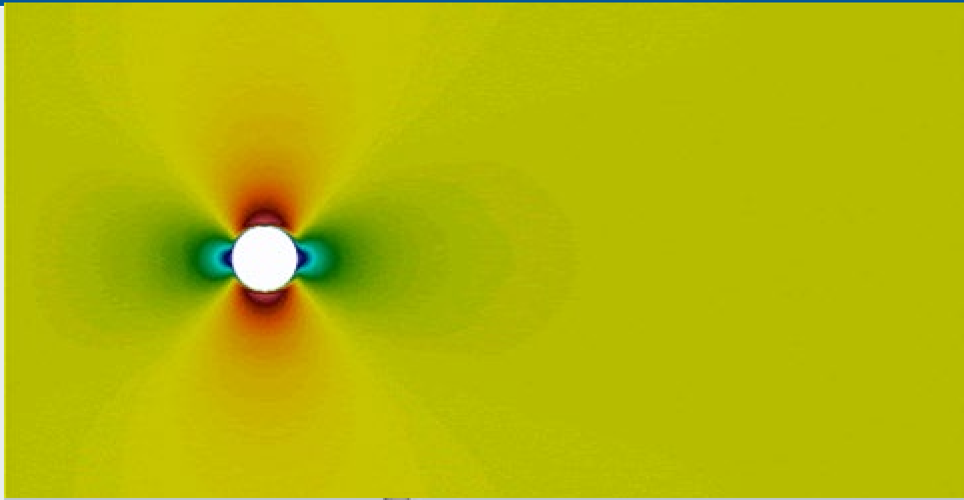
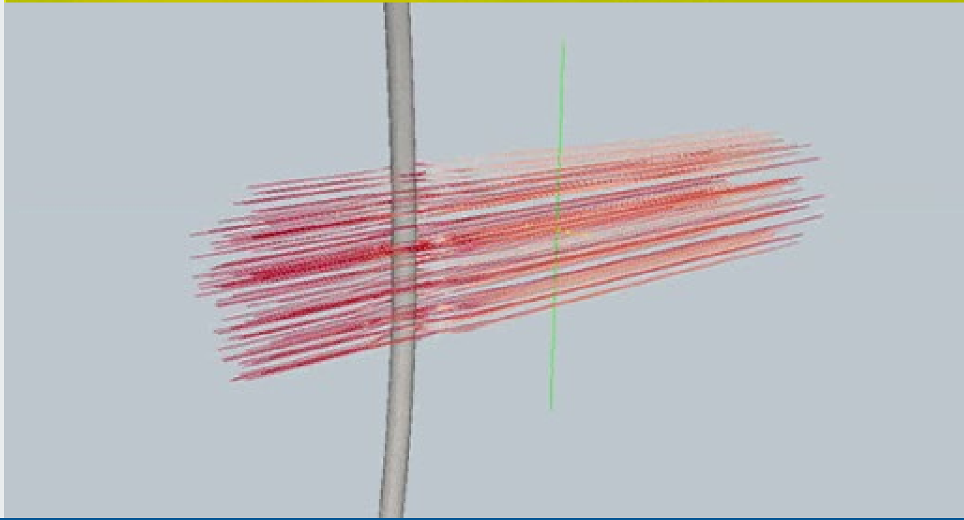
Introduction and Leading Motivations

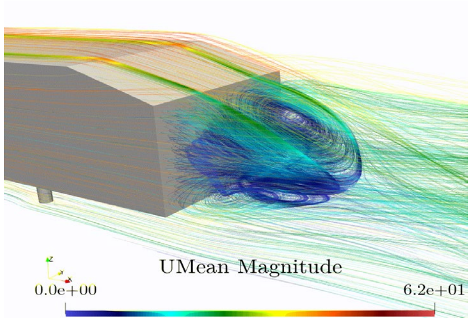
- Need of saving computational resources
- ***Offline-online computational*** procedures



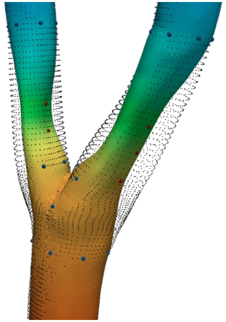


Physical Parametric Differential Problems: Overview

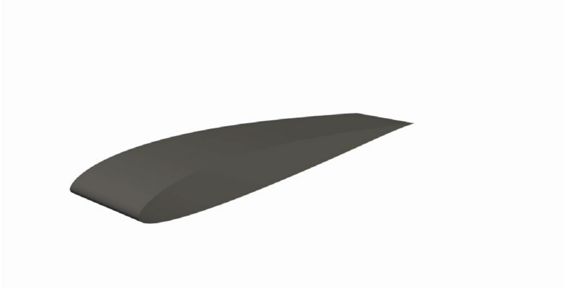
Parametric Differential Problems are ubiquitous in many field of Natural and Applied Sciences from **naval** and **nautical** engineering, to **aeronautical** engineering, **bioengineering**, as well as **industrial** engineering.



automotive



biomedics



aeronautics

Rozza, Gianluigi, Giovanni Stabile, and Francesco Ballarin (2022) eds. Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics. Society for Industrial and Applied Mathematics., CSE series.

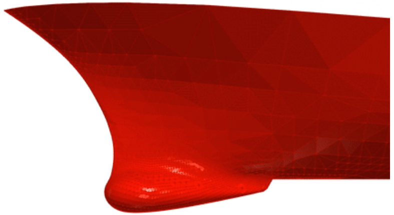
Leading Motivation: CFD challenges

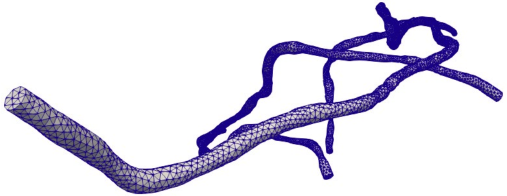
Growing demand of:

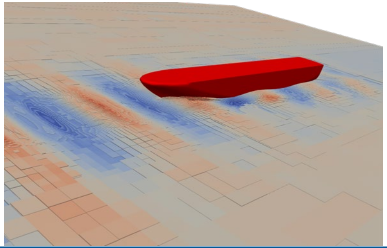
efficient tools	**uncertainty quantification**
parameterized formulations	**real-time** computations

Quickly emerging field of ***Model Order Reduction*** to efficiently **parametrize** and **accelerate** computations

Need of computational collaboration between **Full Order Model (FOM)+HPC** and **Reduced Order Model (ROM)**



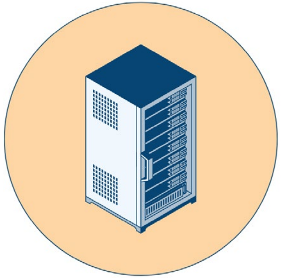




Towards real-time computing

Offline stage

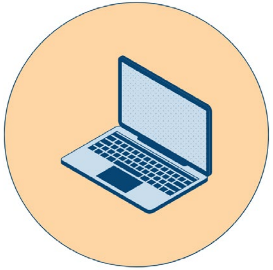
The Full Order Model (FOM)



- Requires *super-computers (HPC)*
- *Expensive* computational resources
- *Several* degrees of freedom
- ***Extremely time-demanding***

Online stage

Reduced Order Model (ROM) techniques

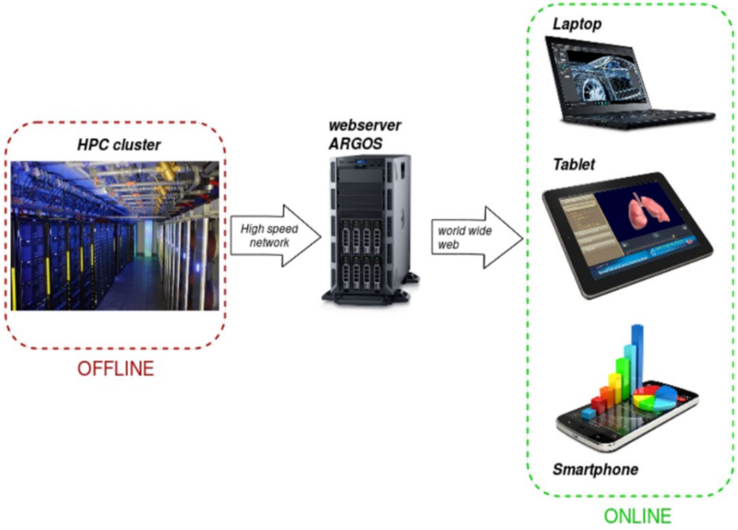


- Needs a *laptop*
- *Small* computational resources
- *Few* degrees of freedom
- ***Fast, real-time computing***

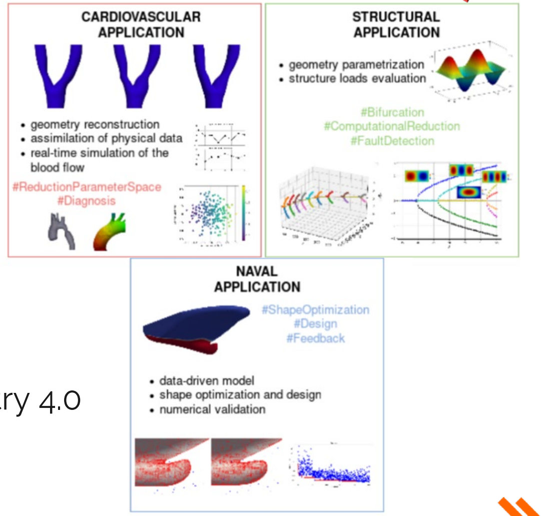
Technology perspective: computational webserver

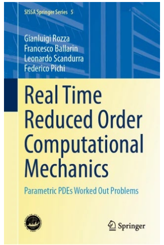
Model order reduction for computational web server: to real world applications (ERC PoC ARGOS):

- `argos-edu.sissa.it`
- `atlas.sissa.it`



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





ARGOS - Computational Webserver

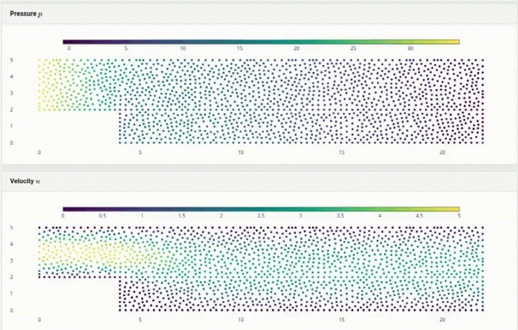
Model order reduction for computational web server: from academic to real world applications

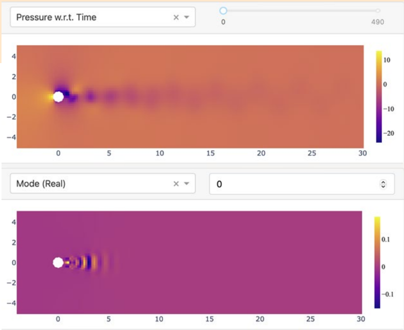
ARGOS

https://argos.sissa.it https://argos-edu.sissa.it

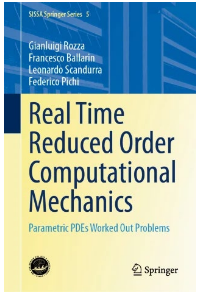
Benchmark applications and **worked out** problems for academia and beyond

POD+Interpolation for Navier-Stokes





DMD



- **real-time** computation
- visualization tool

… and much more!

powered by FAST COMPUTING

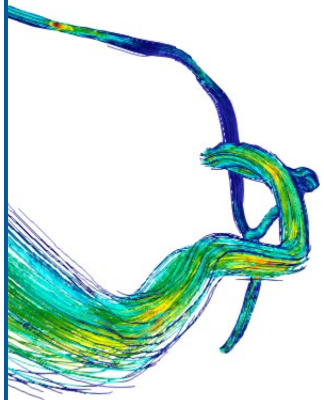
ATLAS - Computational Webserver

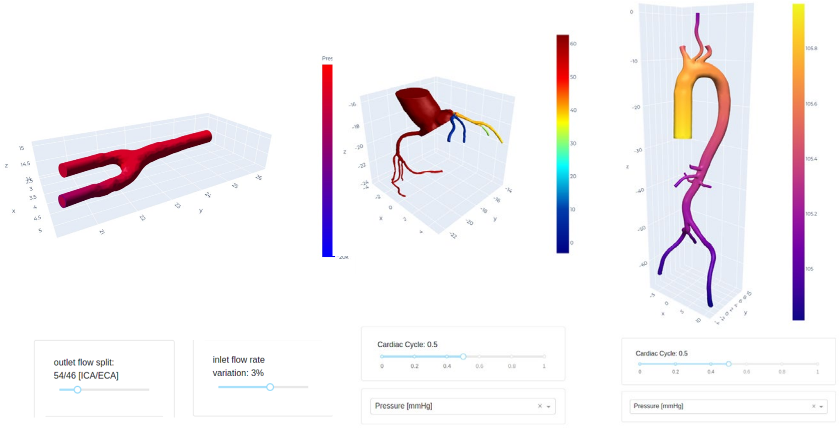
Model order reduction for computational web server: from academic to real world applications

ARGOS

https://atlas.sissa.it

A special focus on **cardiovascular** applications

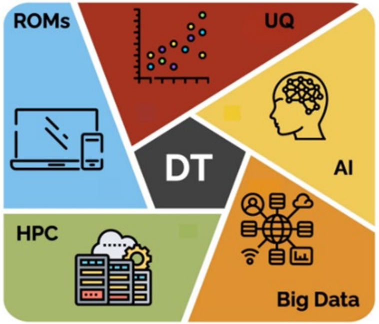




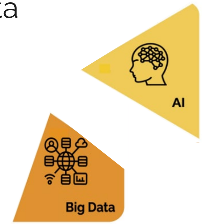
Carotid artery *Coronary arteries* *Aortic model*

powered by FAST COMPUTING

Digital Twin (DT): integration of emerging fields

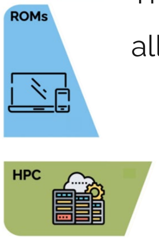


A large amount of data (**Big data**) can be collected



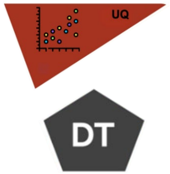
Artificial Intelligence can help to store and organize data.

- By using **black-box models,** AI techniques are able to find **fitting functions**
- It does not require knowledge of 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 **ROMs** allowed to reach better performances for:

- building **Digital Twins** (**DT**) of products and processes;
- **Uncertainty Quantification** (**UQ**);
- Data analytics.



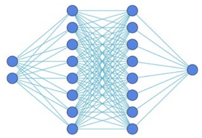
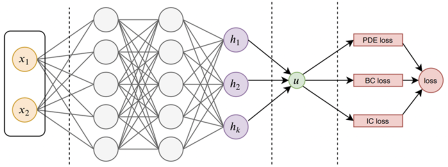
A sustainable perspective (reducing energy consumption, recycling computational works)

SISSA mathLab: our current efforts and perspectives

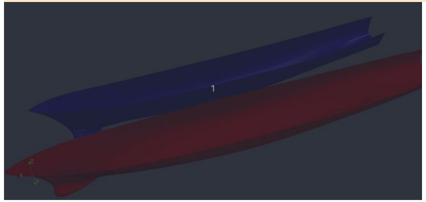
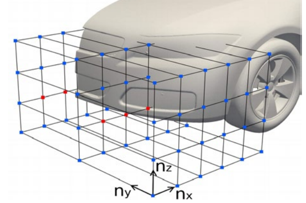
A team developing **Advanced Reduced Order and Surrogate Methods** for parametric PDEs!

SISSA mathLab: our current efforts and perspectives

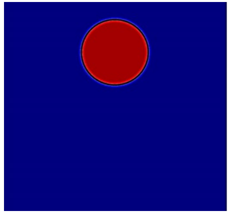
Face and overcome **some limitations** of classic parametric ROM also by means of **Machine Learning**

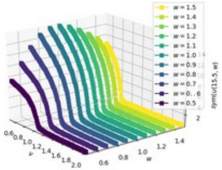
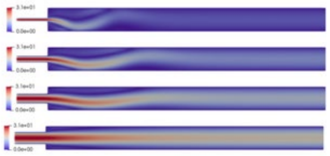
Improve capabilities of ROMs for **more demanding applications** in industrial, medical and applied sciences

CFD as a central topic to enhance broader applications in **multiphysics** and **coupled** settings

Carry out important **methodological developments** with special emphasis on **mathematical modelling**

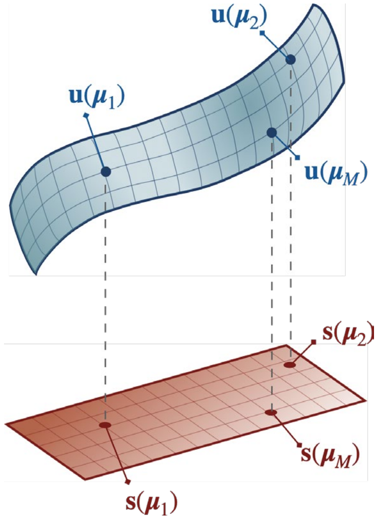
SISSA mathLab: our current efforts and perspectives
Open source libraries: mathlab.sissa.it/cse-software

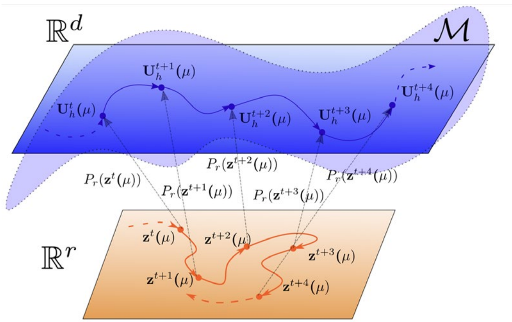
Development of **open-source tools based on surrogate modeling**:

- **ITHACA**, In real Time Highly Advanced Computational Applications, as an add-on to integrate already well established CSE/CFD open-source software
- **RBniCS** as educational initiative (FEM) for newcomer ROM users (training).
- **EzyRB,** data-driven model order reduction for parametrized problems
- **PyDMD,** a Python package designed for Dynamic Mode Decomposition (in collaboration with University of Texas, CERN, and University of Washington)
- **ARGOS A**dvanced **R**educed order modellin**G O**nline computational web server for parametric **S**ystems
- **PINA,** a deep learning library to solve differential equations

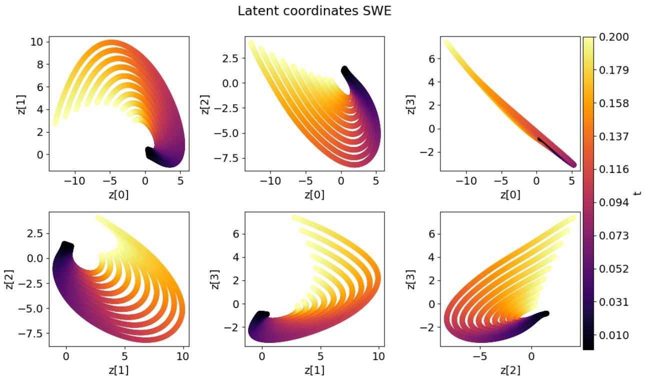
PINA | ITHACA | ITHACA - FV | PyDMD | ITHACA-DG | RBniCS | multiphenics | ARGOS | ATLAS | EZyRB

Reduced Order Models (ROMs)





- ➔ Equation-based or fully data-driven
- ➔ Machine-learning enhanced ROMs
- ➔ Fast Online Phase



Reduced Order Model - Accelerating Numerics

Problem: to find the approximation for an unseen (test) parameter $\boldsymbol{\mu}^\star$

Two macro-types of ROM approach:

Non-Intrusive ROM

- ***purely data-driven*** approach

$$\mathbf{u}(\boldsymbol{\mu}) \xrightarrow{\text{reduce, then approximate}} \mathbf{u}_r(\boldsymbol{\mu}^\star)$$

- no knowledge of the mathematical model needed

Intrusive ROM

- ***equation-based*** approach

$$\mathscr{A}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0 \xrightarrow{\text{reduce, then evolve}} \mathscr{A}_r(\mathbf{u}_r(\boldsymbol{\mu}^\star), \boldsymbol{\mu}^\star) = 0$$

- consolidated mathematical theory

Hesthaven, J. S., Rozza, G., & Stamm, B. (2016). Certified reduced basis methods for parametrized partial differential equations (Vol. 590, pp. 1-131).

Rozza, Gianluigi, Giovanni Stabile, and Francesco Ballarin (2022) eds. Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics. Society for Industrial and Applied Mathematics., CSE series.

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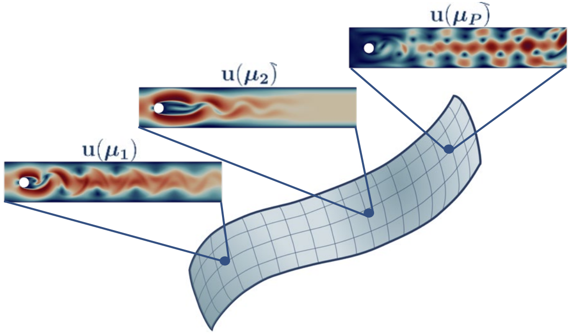
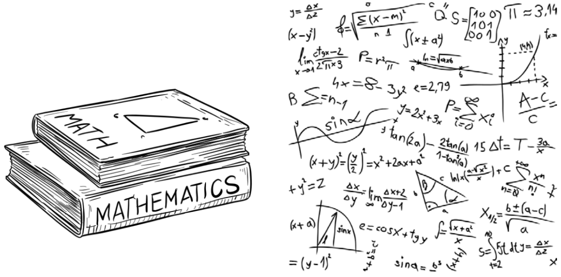
Reduced Order Model - Accelerating Numerics

Recent research goal: integrate data and physics' knowledge

Hybrid ROMs (and Agregated ROMs)



Data collection and integration



Knowledge of the ***equations*** and the ***physical model*** of interest

Rozza, Gianluigi, Giovanni Stabile, and Francesco Ballarin (2022) eds. Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics. Society for Industrial and Applied Mathematics., CSE series.

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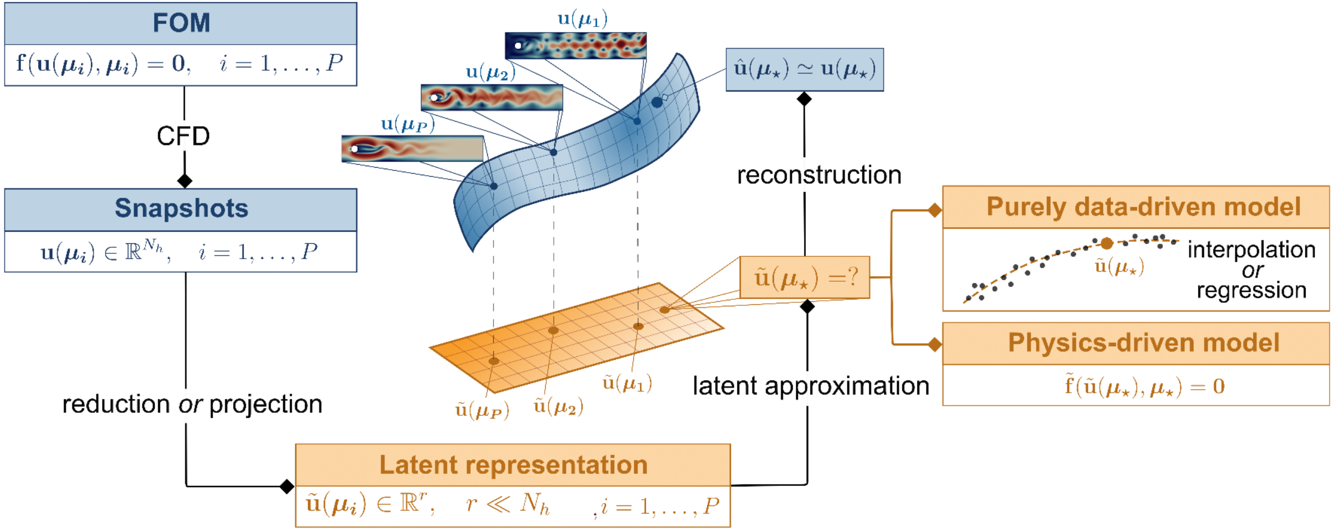
Reduced Order Model - Accelerating Numerics



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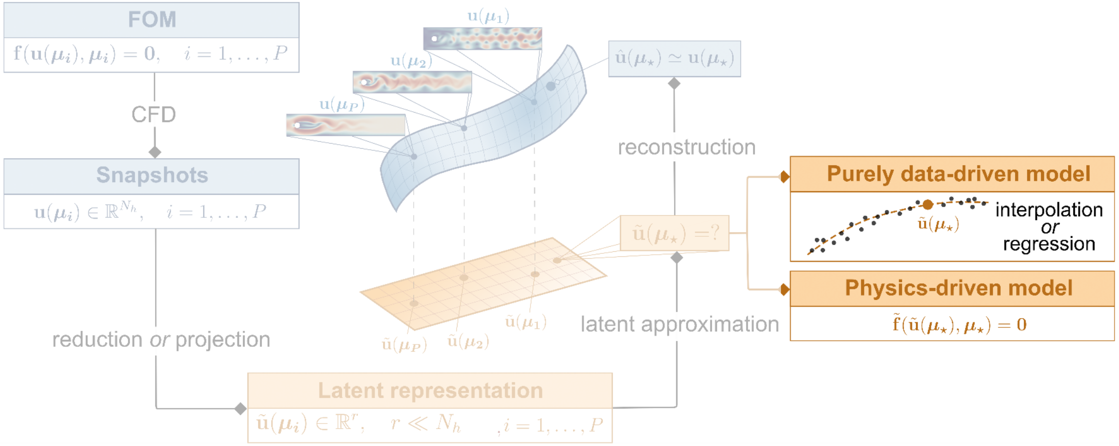
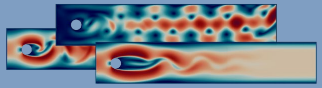
Hybrid ROMs



Goal: integrate

data



and

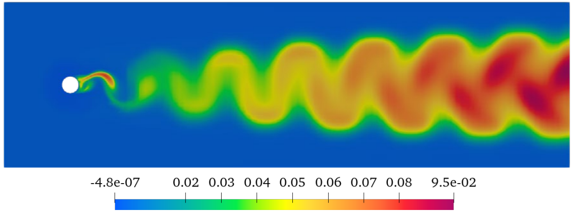
physics $\dot{\mathbf{y}} = f(\mathbf{y}, t)$

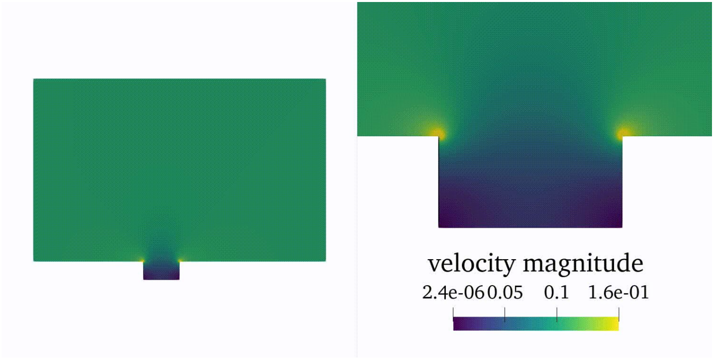
to build an efficient and accurate **hybrid** surrogate model.

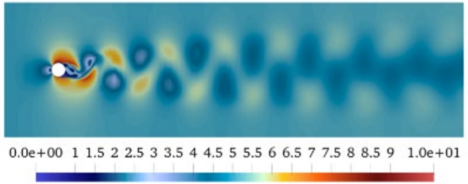
Hybrid data-driven intrusive ROMs for turbulent flows

- ➔ Hybrid approaches for reduced order models
- ➔ How to stabilize and enhance the flows?
- ➔ How to integrate ROMs with machine learning?

Joint work with:
Anna Ivagnes, Giovanni Stabile

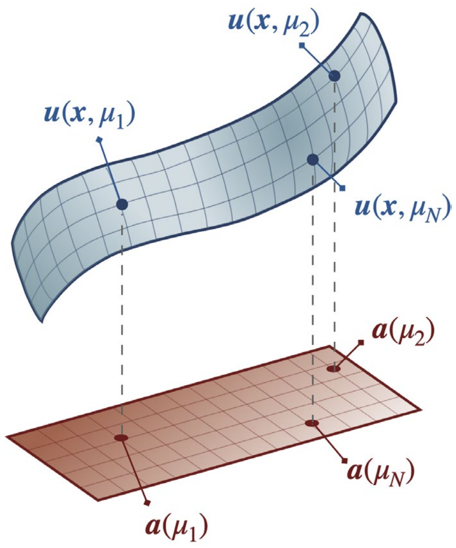






Intrusive ROMs - POD-Galerkin approach

POD principles



Linearity hypothesis

$$u(x,\mu) \sim \sum_{i=1}^{N_u} a_i(\mu)\,\varphi_i(x) \qquad p(x,\mu) \sim \sum_{i=1}^{N_p} b_i(\mu)\,\chi_i(x)$$

$x \in \mathbb{R}^{d \times N_{dof}}$

- ***d:*** dimension
- N_{dof} : degrees of freedom *(several)*

$N_u, N_p \ll N_{dof}$: reduced dimensions for velocity and pressure, chosen ***a priori***

$a = (a_i)_{i=1}^{N_u}$

$b = (b_i)_{i=1}^{N_p}$

vectors of coefficients (**parameter-dependent**)

$(\varphi_i)_{i=1}^{N_u} \quad (\chi_i)_{i=1}^{N_p}$

POD modes (**space-dependent**)

Intrusive ROMs - POD-Galerkin approach

The ***Galerkin*** approach:

- momentum equation projected into the **velocity modes** $$\left(\boldsymbol{\varphi}_i, \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) - \boldsymbol{\nabla} \cdot \nu \left(\boldsymbol{\nabla} \boldsymbol{u} + (\boldsymbol{\nabla} \boldsymbol{u})^T\right) + \boldsymbol{\nabla} p\right)_{L^2(\Omega)} = 0.$$
- continuity equation projected into the **pressure modes** $$(\chi_i, \boldsymbol{\nabla} \cdot \boldsymbol{u})_{L^2(\Omega)} = 0.$$

Reduced ODEs system *(compact form)*

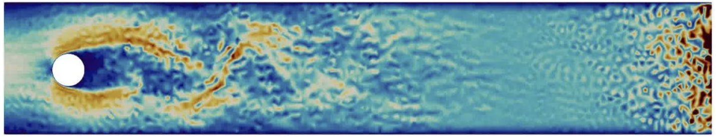
$$\begin{cases} \dot{\mathbf{a}} = \boldsymbol{f}(\mathbf{a}, \mathbf{b}), \\ \boldsymbol{c}(\mathbf{a}) = \mathbf{0}\,. \end{cases}$$

→ dynamical (*cheap*) system to be solved at each *time step*

Stabilized POD-Galerkin ROMs

Stabilization issues in standard ROMs:

- **spurious oscillations**
- ***reduced* inf-sup condition** not fulfilled



Supremizer enrichment

- Enrichment of the velocity POD space with additional N_{sup} modes
- Fulfillment of the inf-sup condition

$$\boldsymbol{a} = (a_i)_{i=1}^{N_u+N_{sup}}$$

$$\boldsymbol{u}(\boldsymbol{x},\boldsymbol{\mu}) = \sum_{i=1}^{N_u+N_{sup}} a_i(\boldsymbol{\mu})\boldsymbol{\varphi}_i(\boldsymbol{x})$$

Pressure Poisson Equation

Replacement of the continuity equation with PPE

- at the ***FOM*** level:

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

- at the ***ROM*** level *(at each time step)*:

$$\boldsymbol{c}(\mathbf{a}) = \mathbf{0} \longrightarrow \boldsymbol{c}(\mathbf{a},\mathbf{b}) = 0$$

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

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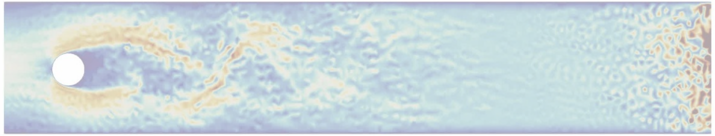

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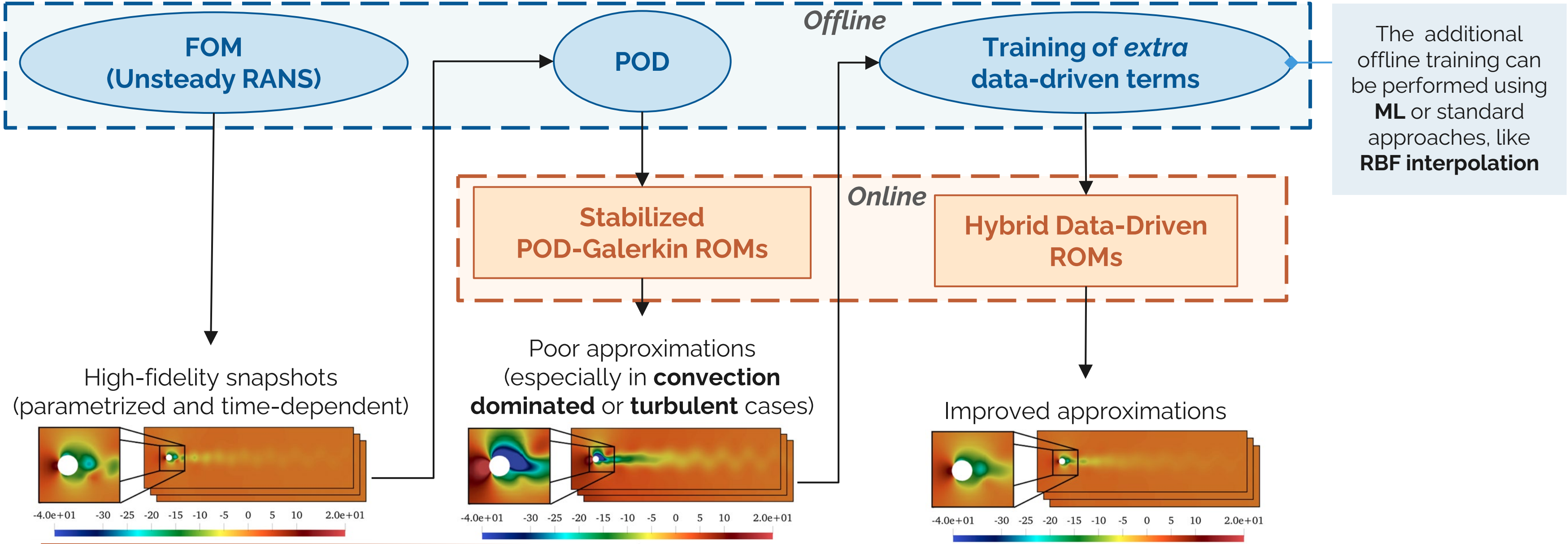
Stabilized ROMs enhanced with data



Ivagnes, A., Stabile, G., & Rozza, G. (2024). Parametric Intrusive Reduced Order Models enhanced with Machine Learning Correction Terms. arXiv preprint arXiv:2406.04169.

Purely DD-ROMs

Purely data-driven approach

WHY

Reintroduce the contribution of the neglected modes in a <u>*LES*</u> fashion

HOW

The procedure to build the *extra-correction* terms

- Choose a reduced dimension ***r*** and a bigger dimension ***d>r***
- Select a stabilization $\mathcal{C}$ operator
- Compute the *exact correction* $\boldsymbol{\tau}^{exact} = \overline{\mathcal{C}(\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_r, \boldsymbol{\varphi}_{r+1}, \ldots, \boldsymbol{\varphi}_d)}^r - \mathcal{C}(\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_r)$
- Create a map for the approximated correction $\boldsymbol{\tau}^{approx} = \boldsymbol{\tau}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{\mu}) = \boxed{\mathcal{M}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{\mu}; \boldsymbol{\theta}_{\mathcal{M}})}$
- Train the map: $\min_{\boldsymbol{\theta}_{\mathcal{M}}} ||\mathcal{M}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{\mu}; \boldsymbol{\theta}_{\mathcal{M}}) - \boldsymbol{\tau}^{exact}||_{L^2}$

PURELY DD-ROM

$$\begin{cases} \dot{\boldsymbol{a}} = \boldsymbol{f}(\boldsymbol{a}, \boldsymbol{b}; \boldsymbol{\mu}^*) + \boldsymbol{\tau}_{\boldsymbol{u}}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{\mu}^*), \\ \boldsymbol{h}_{\mathrm{PPE}}(\boldsymbol{a}, \boldsymbol{b}; \boldsymbol{\mu}^*) + \boldsymbol{\tau}_{\boldsymbol{p}}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{\mu}^*) = \boldsymbol{0}. \end{cases}$$

Ivagnes, A., Stabile, G., Mola, A., Iliescu, T., & Rozza, G. (2023). Pressure data-driven variational multiscale reduced order models. Journal of Computational Physics, 476, 111904.

Physics-based DD-ROMs

Physics-based data-driven approach

WHY

Reintroduce the turbulence modeling in ROMs in a *RANS* fashion

HOW

Modeling the reduced eddy viscosity

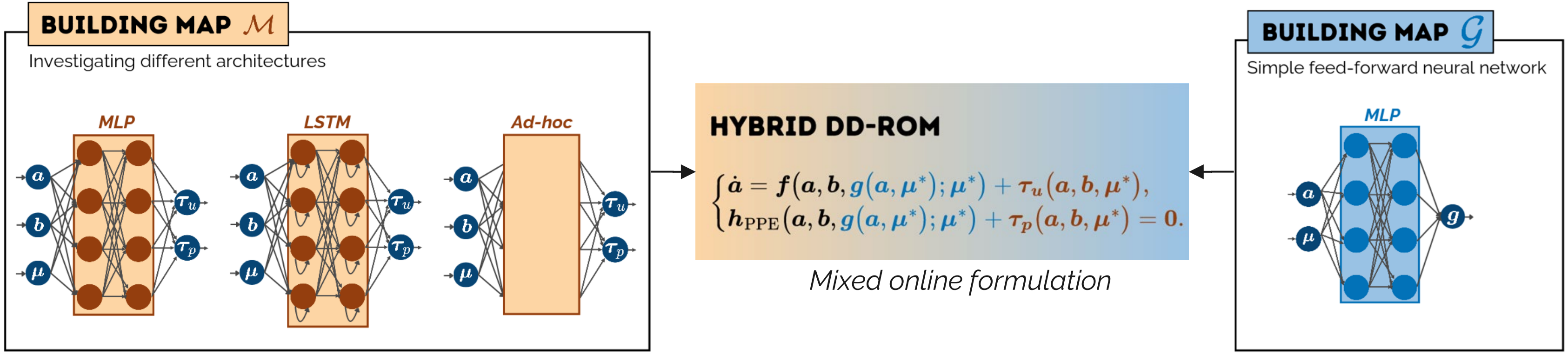
- Choose a reduced dimension for the eddy viscosity N_{ν_t}
- Extract the eddy viscosity modes $(\eta_i(\boldsymbol{x}))_{i=1}^{N_{\nu_t}}$ such that: $\nu_t(\boldsymbol{x}, \boldsymbol{\mu}) \simeq \sum_{i=1}^{N_{\nu_t}} g_i(\boldsymbol{\mu})\eta_i(\boldsymbol{x})$
- Compute the *projected coefficients* $\boldsymbol{g}^{exact}$
- Create a map for the approximated correction $\boldsymbol{g}^{approx} = \boldsymbol{g}(\boldsymbol{a}, \boldsymbol{\mu}) = \mathcal{G}(\boldsymbol{a}, \boldsymbol{\mu}; \boldsymbol{\theta}_{\mathcal{G}})$
- Train the map: $\min_{\boldsymbol{\theta}_{\mathcal{G}}} ||\mathcal{G}(\boldsymbol{a}, \boldsymbol{\mu}; \boldsymbol{\theta}_{\mathcal{G}}) - \boldsymbol{g}^{exact}||_{L^2}$

PHYSICS-BASED DD-ROM

$$\begin{cases} \dot{\boldsymbol{a}} = \boldsymbol{f}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{g}(\boldsymbol{a}, \boldsymbol{\mu}^*); \boldsymbol{\mu}^*), \\ \boldsymbol{h}_{\text{PPE}}(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{g}(\boldsymbol{a}, \boldsymbol{\mu}^*); \boldsymbol{\mu}^*) = \boldsymbol{0}. \end{cases}$$

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

Machine learning maps



Purely data-driven training
(aimed to reintegrate missing modes)

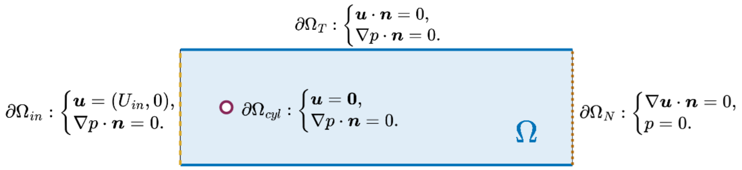
Physics-based data-driven training
(aimed to reintegrate turbulence)

Ivagnes, A., Stabile, G., & Rozza, G. (2024). Parametric Intrusive Reduced Order Models enhanced with Machine Learning Correction Terms. arXiv preprint arXiv:2406.04169.

Ivagnes, A., Stabile, G., Mola, A., Iliescu, T., & Rozza, G. (2023). Hybrid data-driven closure strategies for reduced order modeling. Applied Mathematics and Computation, 448, 127920.

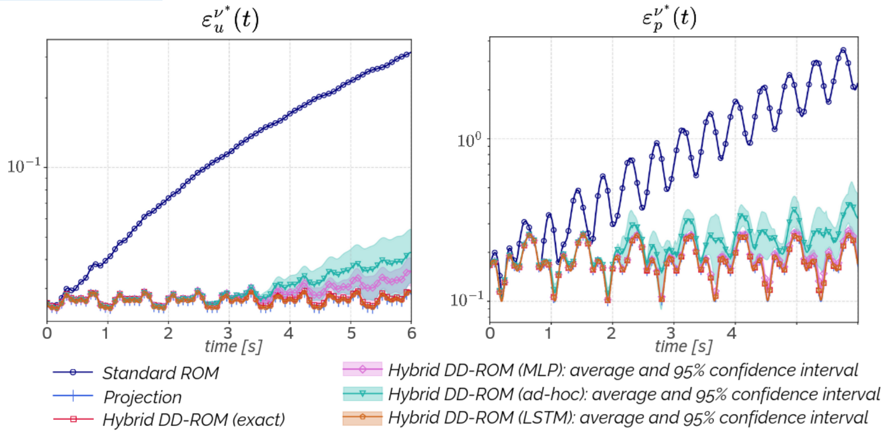
Numerical results

Test case: *periodic flow past a cylinder*
Parameters: *time and Reynolds number*
Number of modes**:** ***3*** *for velocity, pressure and eddy viscosity*



ERROR ANALYSIS
(for a test parameter and in time extrapolation)

- $$\varepsilon_u^{\nu^*}(t) = \frac{\|\boldsymbol{u}_{\mathrm{FOM}}^{\nu^*}(t) - \boldsymbol{u}_{\mathrm{ROM}}^{\nu^*}(t)\|_{L^2(\Omega)}}{\|\boldsymbol{u}_{\mathrm{FOM}}^{\nu^*}(t)\|_{L^2(\Omega)}}$$
- $$\varepsilon_p^{\nu^*}(t) = \frac{\|p_{\mathrm{FOM}}^{\nu^*}(t) - p_{\mathrm{ROM}}^{\nu^*}(t)\|_{L^2(\Omega)}}{\|p_{\mathrm{FOM}}^{\nu^*}(t)\|_{L^2(\Omega)}}$$

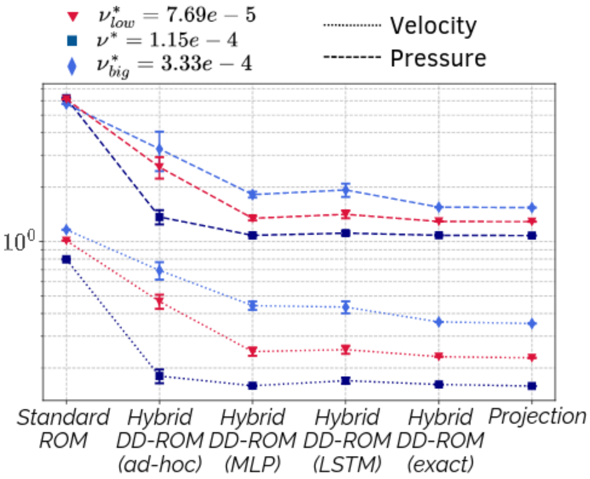


Ivagnes, A., Stabile, G., & Rozza, G. (2024). Parametric Intrusive Reduced Order Models enhanced with Machine Learning Correction Terms. arXiv preprint arXiv:2406.04169.

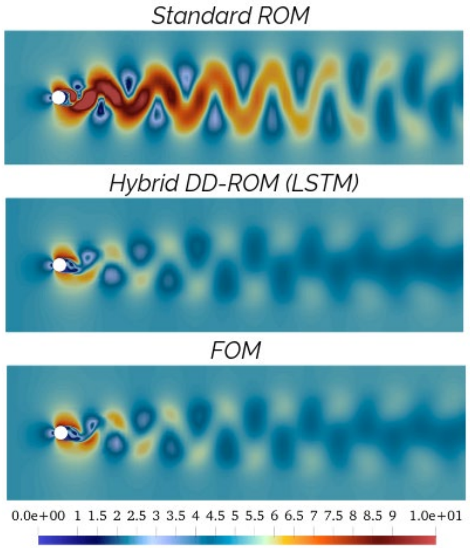
Graphical results

ANALYSIS OF GLOBAL PERFORMANCE

- *Computation of the errors' **time integrals***
- ***Graphical** velocity fields at the final instance of the online ROM simulation*



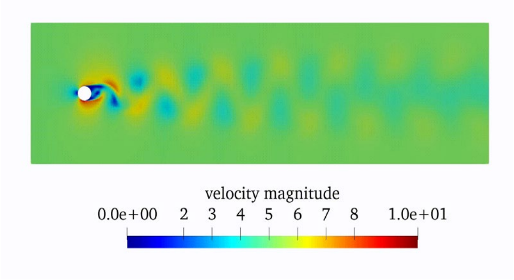
Time integrals of relative errors



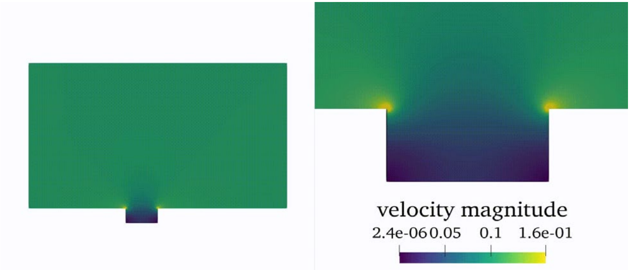
Ivagnes, A., Stabile, G., & Rozza, G. (2024). Parametric Intrusive Reduced Order Models enhanced with Machine Learning Correction Terms. arXiv preprint arXiv:2406.04169.

Numerical results: the test cases

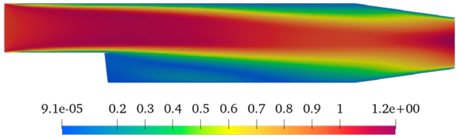
Unsteady flow past a cylinder with parameters (ν, t)

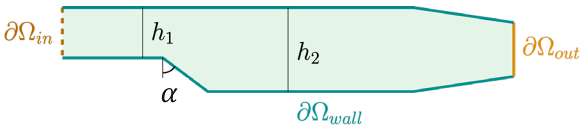


Unsteady channel-driven cavity flow with parameters (ν, t)



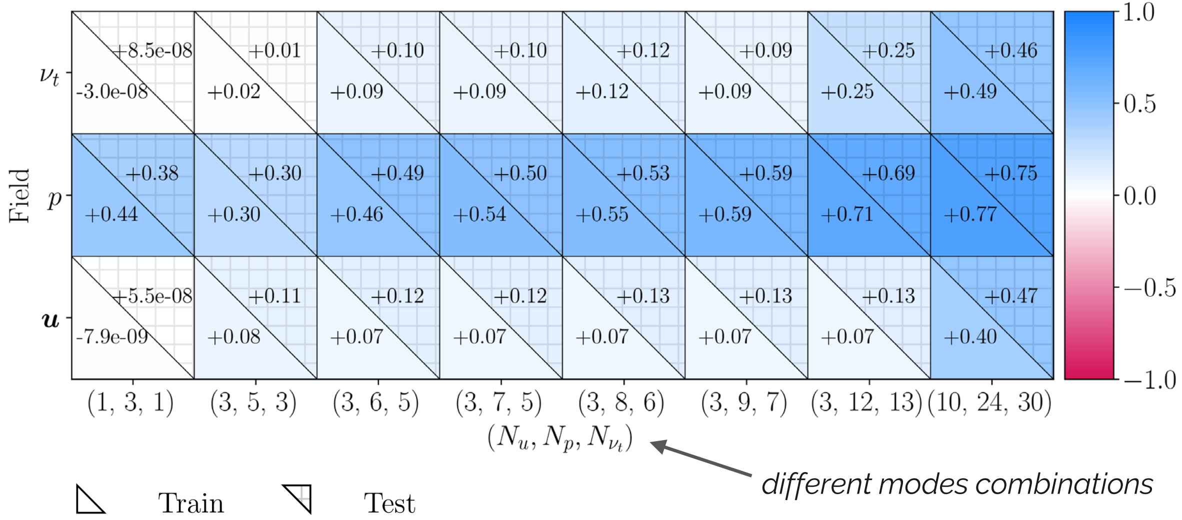
Steady backward-facing step flow with geometrical parameters (α, h_1, h_2)





Numerical results: the flow past a cylinder

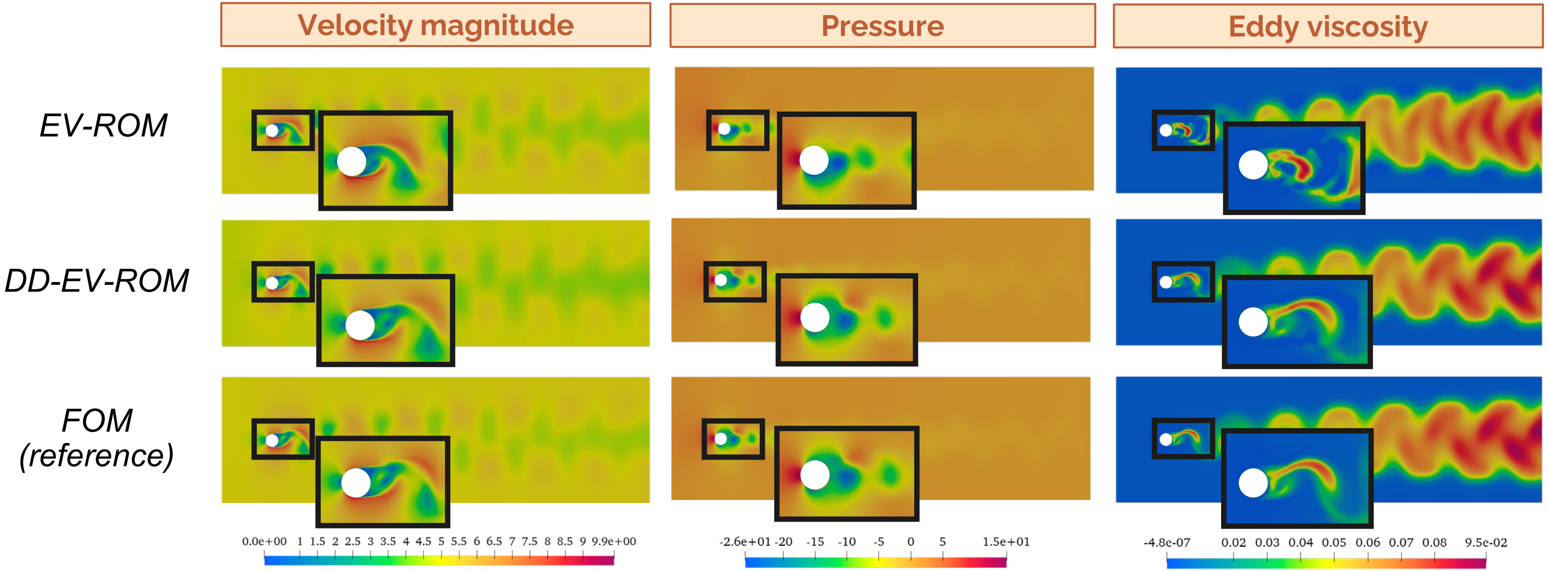
Average gain in the relative error of ***DD-EV-ROM*** with respect to the state-of-the-art baseline ***EV-ROM***



- Improvement of the accuracy especially for the ***pressure***: we introduce a ***dedicated pressure closure***
- Good predictive performance in all modal regimes

Numerical results: the flow past a cylinder

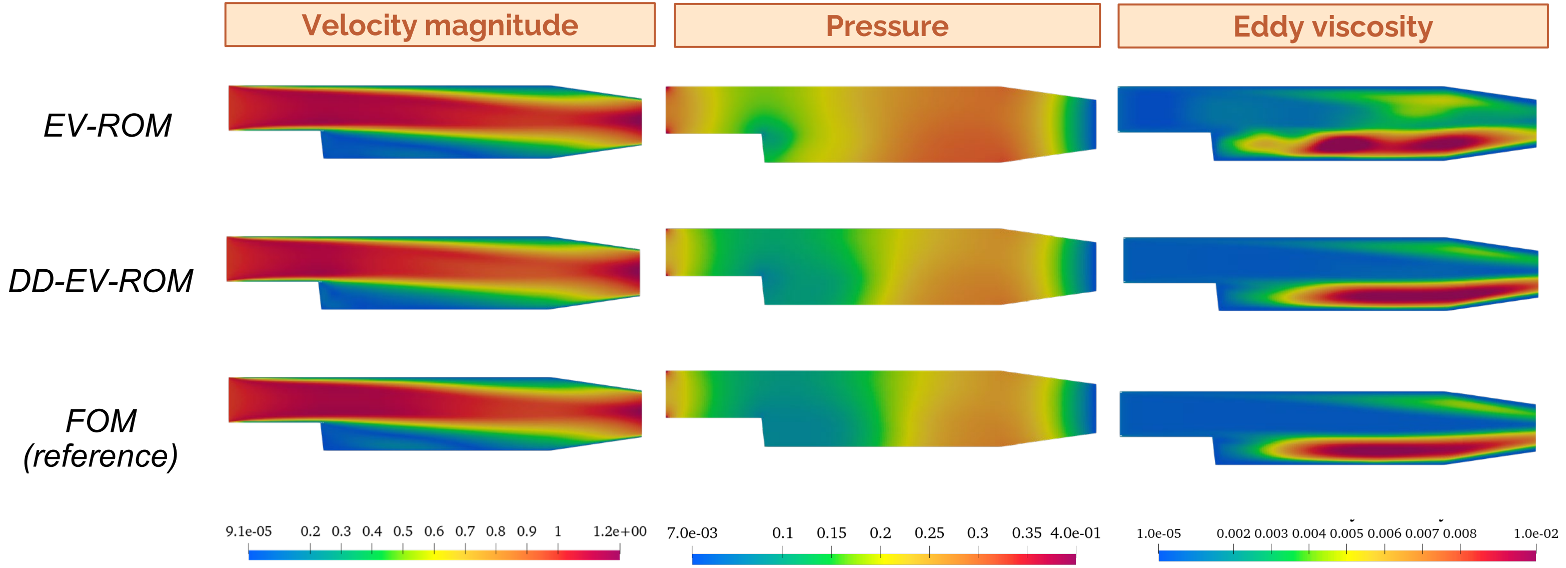
Graphical results for $(N_u, N_p, N_{\nu_t}) = (10, 24, 30)$ for a test parameter



Improved accuracy and fields' reconstruction in the novel ***DD-EV-ROM***

Numerical results: the backward-facing step

Graphical results for $(N_u, N_p, N_{\nu_t}) = (4, 5, 20)$ for a test parameter



Improved accuracy and fields' reconstruction in the novel ***DD-EV-ROM***

Intrusive ROMs for turbulent and compressible problems

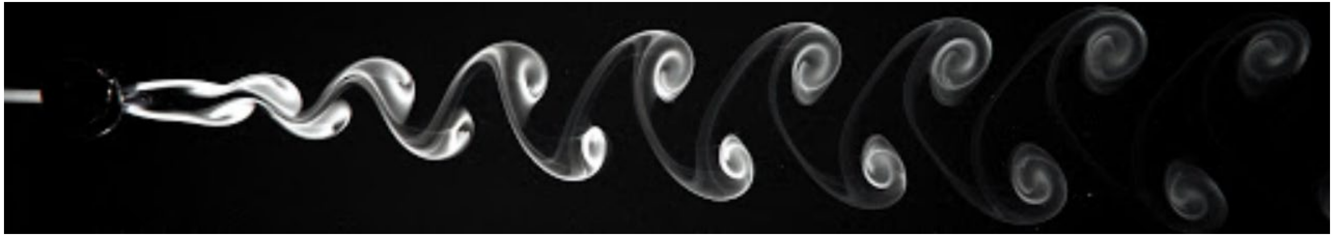
- How to improve ROMs in compressible flows
- ROM segregated methods
- FOM-ROM consistency

Joint work with:
Matteo Zancanaro, Giovanni Stabile

Overview of the physical problem of interest

- The scope of this work is the **resolution of parametric computational fluid dynamics problems** where an unaffordable computational cost is required to obtain accurate solutions;

- Applications of interest are spread over different fields and scales: **aerospace engineering**, **automotive industry**, **nautical studies** or **environmental fields**.



The analytical model for compressible flows

What is this problem characterized by?

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

The Favre averaged Navier–Stokes Equations

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

The Favre averaging rule

$$\tilde{\Phi} = \frac{\overline{\rho\Phi}}{\bar{\rho}}, \qquad \Phi = \tilde{\Phi} + \Phi''.$$

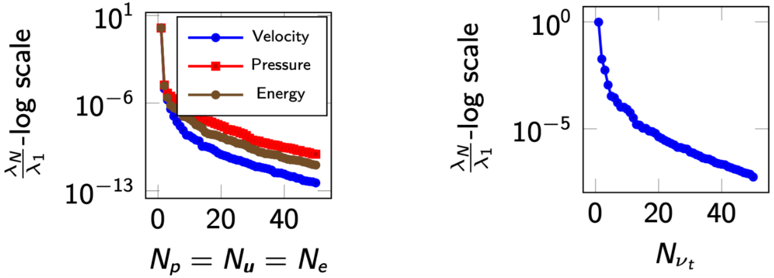
$$\boldsymbol{u} = \tilde{\boldsymbol{u}} + \boldsymbol{u}'', \qquad e = \tilde{e} + e''.$$

Results - ROM with physical parameterization

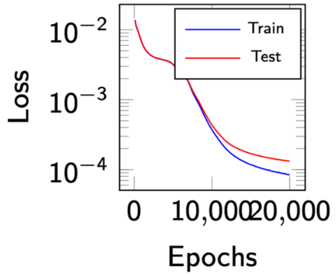
Test case: flow around a **NACA 0012** airfoil where the **viscosity** is parametrized.

Data of the problem:

- $\mu \in [10^{-5}, 10^{-2}]$, $\mu_{on} = 1.2 \times 10^{-3}$;
- Mach $= 0.73$;
- $Re \in 2.92 \times [10^4, 10^7]$;
- number of offline snapshots: $N_{off} = 50$;
- activation function of the neural network: Tanh ;
- number of epochs for training of the neural network: 2×10^3 epochs;
- reduced number of modes: $N_u = N_p = N_e = 20$;
- reduced number of modes for eddy viscosity: $N_{\nu_t} = 30$.



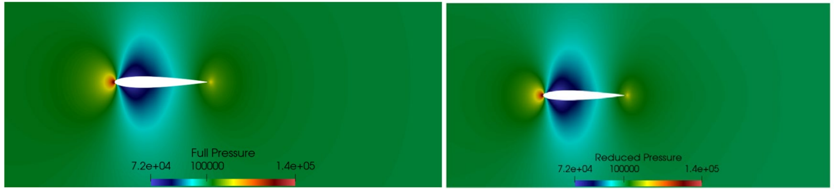
Eigenvalues decay for all the fields of interest



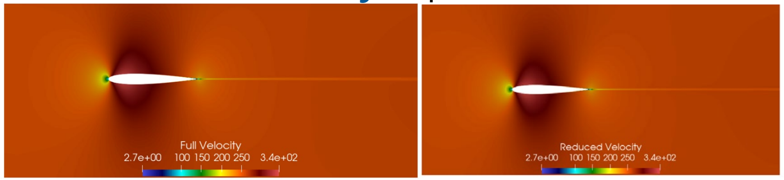
Loss of the neural network used for eddy viscosity coefficients

Results - ROM with physical parametrization

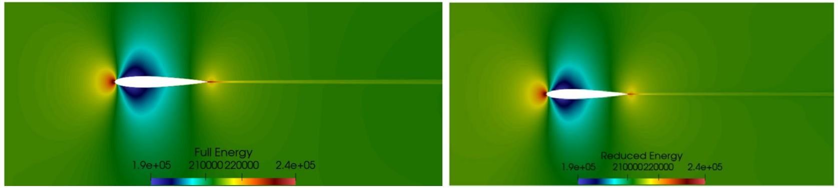
Test case: flow around a **NACA 0012** airfoil where the **viscosity** is parametrized.



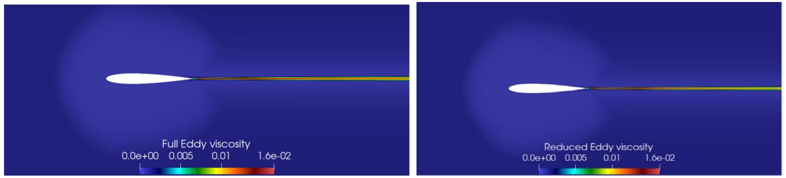
FOM-ROM (pressure)



FOM-ROM (velocity)



FOM-ROM (energy)

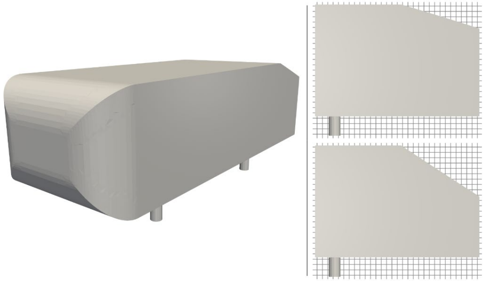


FOM-ROM (eddy viscosity)

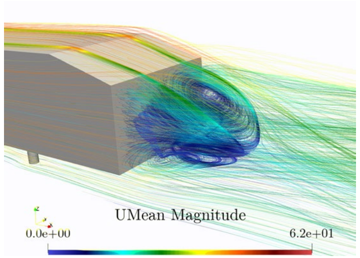
Zancanaro, M., Stabile, G., & Rozza, G. *Segregated methods for reduced order models, 2023.*

ROM with geometrical parameterization

Ahmed body test case with varying slant angles



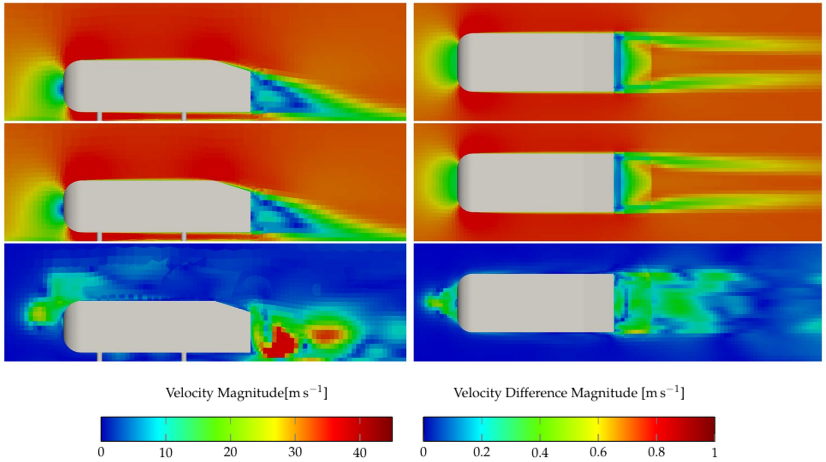
Isogeometric view of the Ahmed body and side views for minimum and maximum slant angles



FOM

ROM

Absolute error FOM-ROM

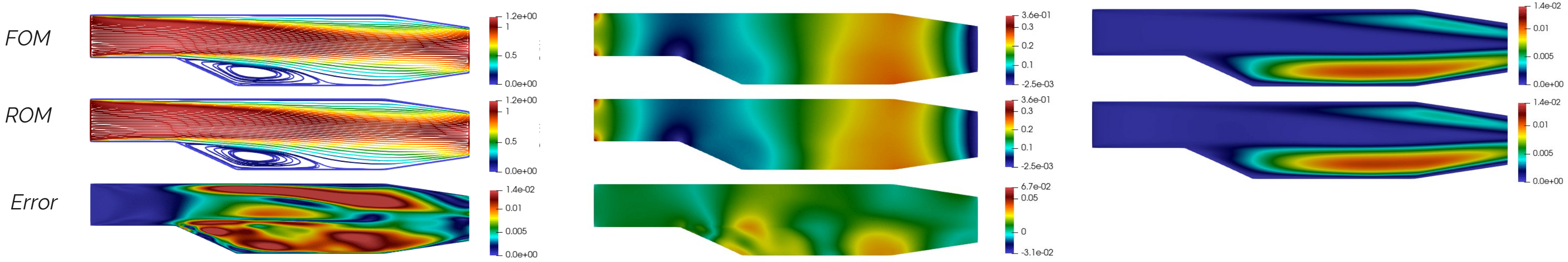


Zancanaro, M., Mrosek, M., Stabile, G., Othmer, C., & Rozza, G. (2021). *Hybrid neural network reduced order modelling for turbulent flows with geometric parameters.* Fluids, 6(8), 296.

ROM with geometrical parameterization

Backstep test case: the step is constructed as a **moving boundary** so that the slope β can varies

Geometry deformation in backstep channel



***Velocity** field FOM-ROM comparison*

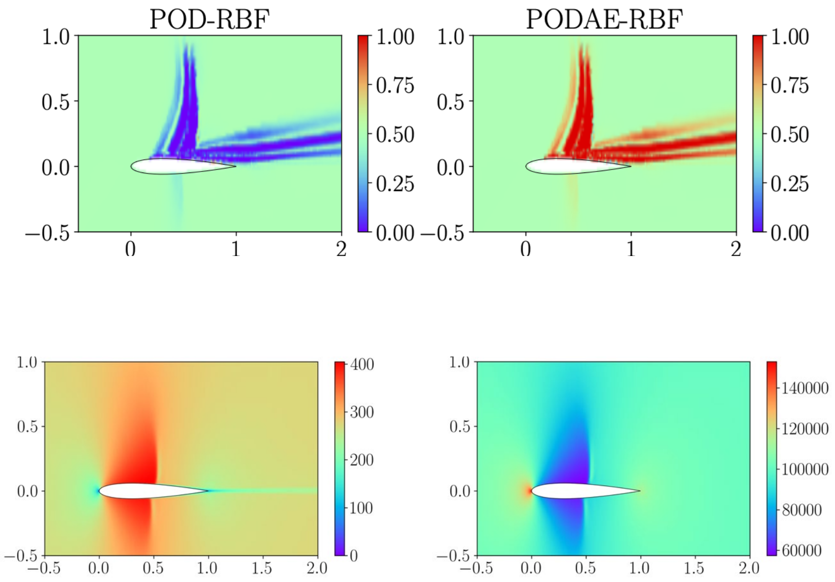
***Pressure** field FOM-ROM comparison*

***Eddy viscosity** field FOM-ROM comparison*

Zancanaro, M., Mrosek, M., Stabile, G., Othmer, C., & Rozza, G. (2021). *Hybrid neural network reduced order modelling for turbulent flows with geometric parameters.* Fluids, 6(8), 296.

Non-Intrusive ROMs enhanced with aggregation models

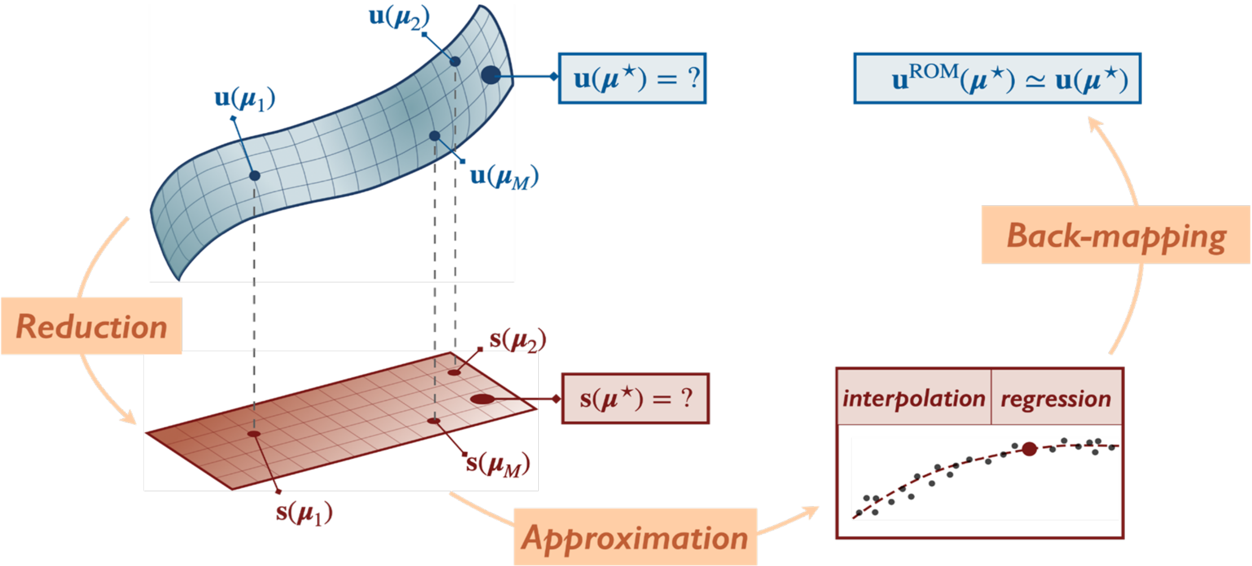
➔ Exploit predictions of different ROMs
➔ *Automatically* deduce the best model
➔ Associate space-dependent weights to every ROM in a *model mixture*



Joint work with:
Anna Ivagnes, Niccoló Tonicello,
Paola Cinnella *(Sorbonne University)*

Non-intrusive ROM

ROM approximate the high dimensional solution manifold by dimensionality reduction and perform interpolation to find the prediction for unseen parameters.

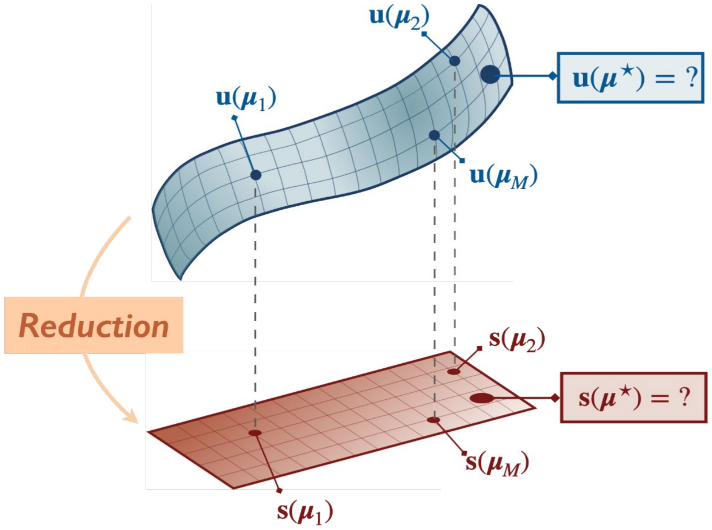


Leading motivation for *mixed-ROMs*

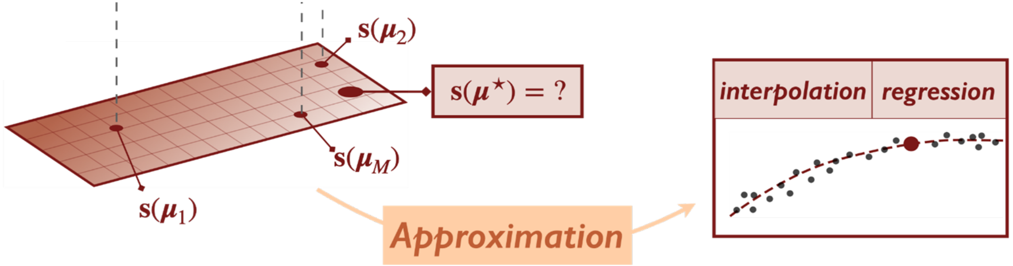
Individual ***reduction*** approaches are not always accurate:

- the **POD** as a **linear** reduction is inaccurate in ***advection-dominated problems*** (high Reynolds parameter) and ***nearby discontinuities*** (i.e. shocks)

- the **AE (AutoEncoder)** as a **nonlinear** approach is more accurate close to shocks but inaccurate in ***smooth regions***



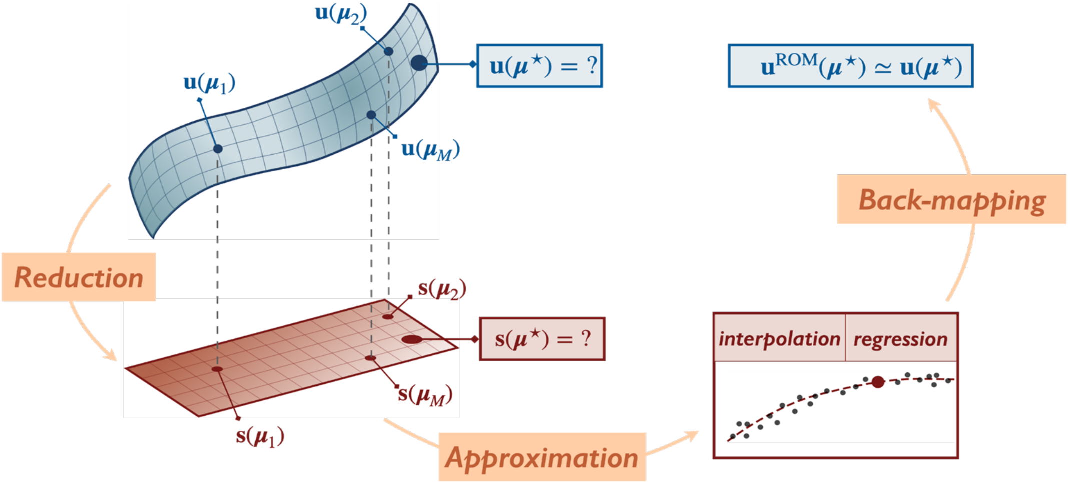
Leading motivation for *mixed-ROMs*



Individual ***approximation*** techniques are not always accurate:

- the **RBF (Radial Basis Function Interpolation)** is characterized by ***smooth interpolants***, but is ***sensitive to the basis function*** chosen;
- the **GPR (Gaussian Process Regression)** is characterized by ***automated hyperparameter tuning*** but it is ***sensitive to noisy data***;
- the **ANN (Artificial Neural Network)** can capture ***complex relationships*** in data but it is ***expensive and hard to train***.

Leading motivation for *mixed-ROMs*



Build a **database of ROMs**, combined in a ***mixed-ROM***, whose prediction is the convex combination of the individual ROMs in the database.

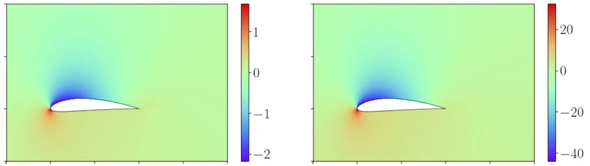
de Zordo-Banliat, M., Dergham, G., Merle, X., & Cinnella, P. (2024). *Space-dependent turbulence model aggregation using machine learning. Journal of Computational Physics*, *497*, 112628.

Cherroud, S., Merle, X., Cinnella, P., & Gloerfelt, X. (2023). *Space-dependent aggregation of data-driven turbulence models. arXiv preprint arXiv:2306.16996*.

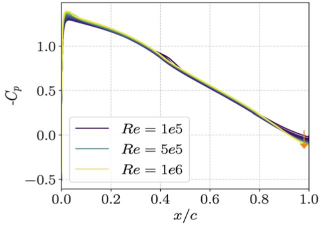
Pipeline of aggregation-ROMs

1. ***Run the FOM and build a database***
2. ***Divide the database into training, validation and test database***

Test case 1



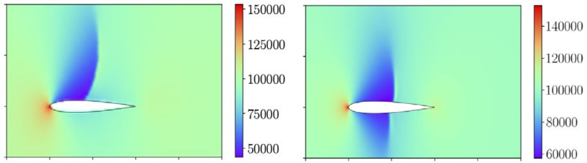
Two pressure snapshots



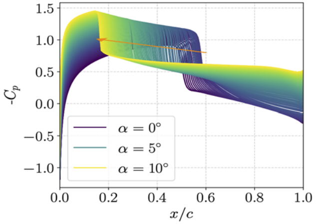
Pressure coefficient

Reynolds number varies in interval **[1e5, 1e6]**

Test case 2



Two pressure snapshots



Pressure coefficient

Angle of attack varies in interval **[0, 10] degrees**

More challenging test case: the shock position varies a lot!

Pipeline of aggregation-ROMs

Training ROMs

3. *Compute different ROMs in the training database*

Set of ROMs: $\mathscr{M} = \{M_1, M_2, \ldots, M_{n_M}\}$

- M_i is a non-intrusive ROM
- $\delta^{(i)}(\eta)$ is the prediction of M_i
- η is the set of parameters (spatial/physical)

Fields approximated with ROM:

- 1D *pressure*/*wall shear stress* on airfoil
- 2D *pressure*/*velocity magnitude* around airfoil

ROMs considered in $\mathscr{M}$:

- POD-RBF
- POD-GPR
- POD-ANN

- AE-RBF
- AE-GPR
- AE-ANN

→ In the case of 2D fields **AE** is replaced with **PODAE** to gain computational time

Pipeline of aggregation-ROMs

The model mixture

4. Compute the weights associated to ROMs in the validation database

Prediction of the aggregation model:

$$\delta^{(mixed)}(\eta) = \sum_{i=1}^{n_M} w_i(\eta)\delta^{(i)}(\eta)$$

How to compute the weights?

ROM prediction ↓ $\delta^{(i)}(\eta_d)$ — FOM Snapshot ↓ $\overline{\delta}_d$

$$\forall M_i : \quad w_i(\eta_d) = \frac{g_i(\eta_d)}{\sum_{j=1}^{n_M} g_j(\eta_d)}, \quad g_i(\eta_d) = exp\left(-\frac{1}{2}\frac{(\delta^{(i)}(\eta_d) - \overline{\delta}_d)^2}{\sigma^2}\right)$$

$(\overline{\delta}_d)_{i=1}^{N_\delta}$ Snapshots in ***validation set***

Pipeline of aggregation-ROMs

Testing the method

5. *Predict the weights in the test database*

DATA (from validation set) —Regression (RF)→ **UNKNOWN** (in test set)

$(g_i(\eta_d))_{d=1}^{N_\delta} \quad \forall M_i$ $\qquad$ $g_i(\eta^*) \quad \forall M_i$

6. *Test the method for unseen configurations*

$$\delta^{(mixed)}(\eta^*) = \sum_{i=1}^{n_M} w_i(\eta^*)\,\delta^{(i)}(\eta^*)$$

UQ analysis

Consider the prediction as a random variable

Expected value:

$$E[\hat{\delta}(\eta)] = \delta^{(mixed)}(\eta) = \sum_{i=1}^{n_M} w_i(\eta)\delta^{(i)}(\eta)$$

Variance:

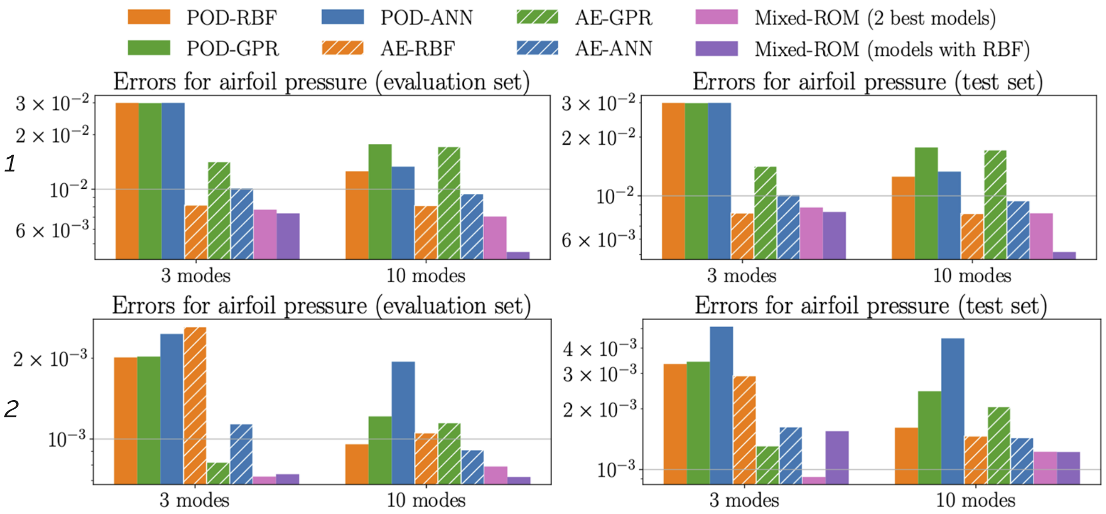
$$Var[\hat{\delta}(\eta)] = \sum_{i=1}^{n_M} w_i(\eta)\left(\delta^{(i)}(\eta) - E[\hat{\delta}(\eta)]\right)^2$$

Results of aggregation model

Relative errors for 1D airfoil pressure

Test case 1

Test case 2



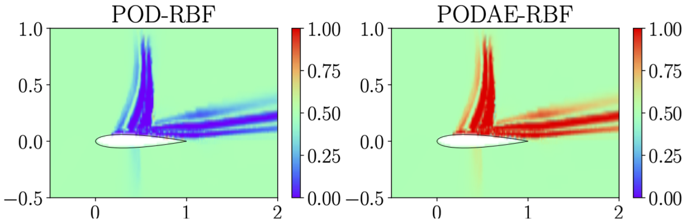
- ***Latent dimensions***: 3 and 10
- Improvement of accuracy in:
  - **validation set** (guaranteed by mathematical law)
  - **test set** (depends on the regression model)

Ivagnes, A., Tonicello N., Cinnella P., and Rozza G., *Enhancing non-intrusive Reduced Order Models with space-dependent aggregation methods*, Acta Mechanica, 2024.

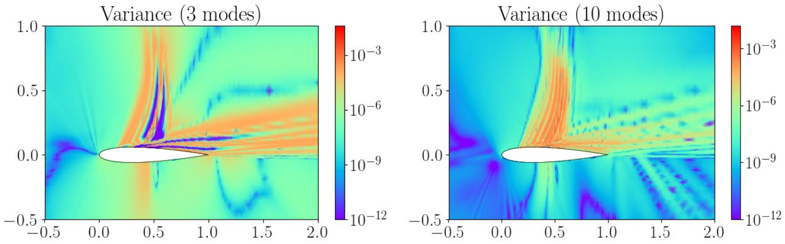
Results of aggregation model

Results for a test parameter (test case 2)

The weights are higher for the AE **nearby the shock position** and **nearby the wake**, where the nonlinear reduction is more accurate



Weights spatial distribution (3 modes)



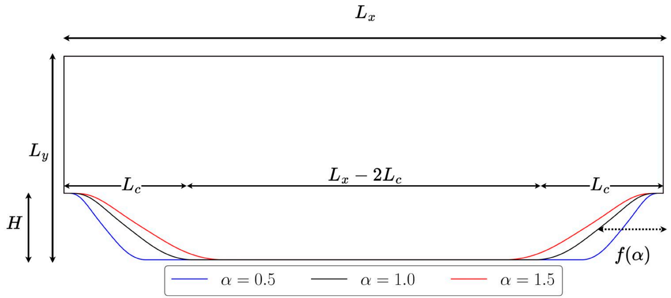
The **variance** gives information on

- *consensus* among ROMs in space
- *deviation* of mixed-ROMs with respect to individual models

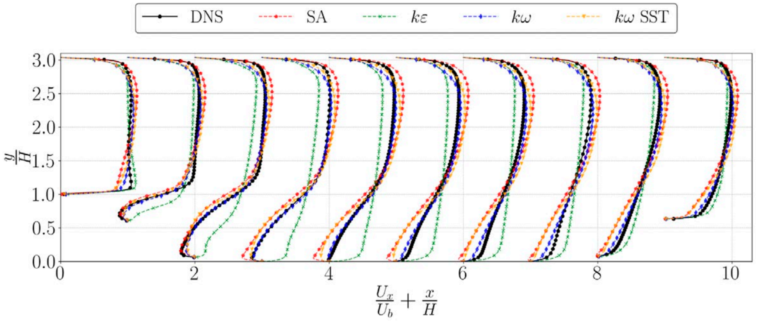
Ivagnes, A., Tonicello N., Cinnella P., and Rozza G., *Enhancing non-intrusive Reduced Order Models with space-dependent aggregation methods,* accepted in Acta Mechanica, 2024.

Towards multi-fidelity: motivation

The test case: flow over periodic hills with parameterized geometry



Periodic hills geometry: our parameters are L_x and α.



Prediction of different RANS models for a specific geometry.

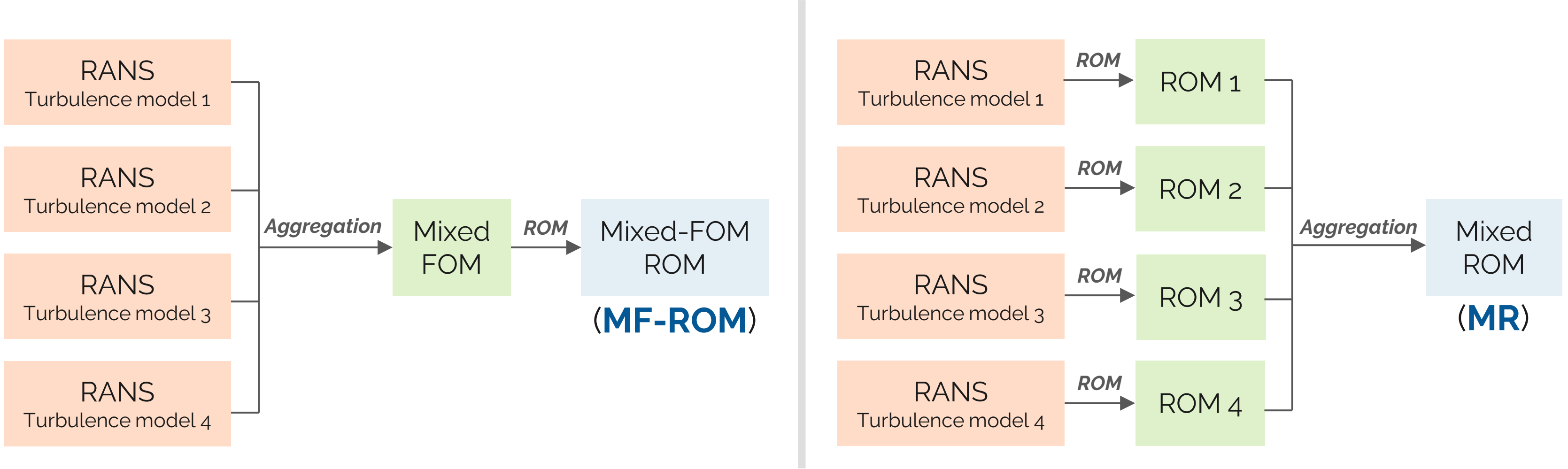
- We only have access to ***11 DNS snapshots***
- We collect different sets of ***RANS snapshots*** using different ***turbulence models***

The RANS simulations perform in different ways across the domain: **this is the ideal case for aggregation**.

Zappi, P., Ivagnes A., Tonicello P., and Rozza G., *Aggregation pipelines using high and low-fidelity models in fluid dynamics*, in preparation.

Towards multi-fidelity: two aggregation pipelines

<u>Idea</u>: integrate the efficiency of ROMs *upstream* or *downstream*

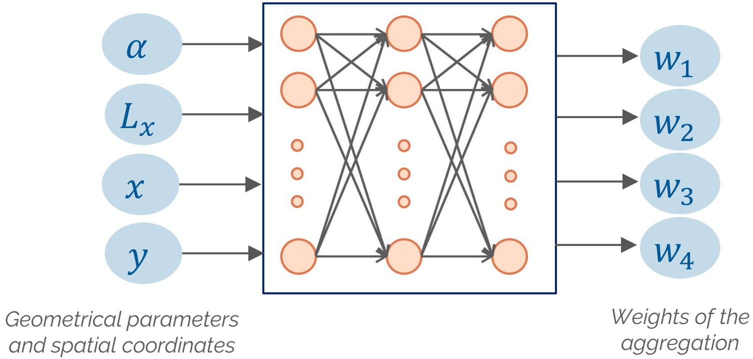


Zappi, P., Ivagnes A., Tonicello P., and Rozza G., *Aggregation pipelines using high and low-fidelity models in fluid dynamics*, in preparation.

Towards multi-fidelity: aggregation results

Aggregation strategies

1. Compute the weights in train set using the standard aggregation formula, and use ***KNN regressor*** in test
2. Use an ***ANN*** to learn (in train set) and infer (in test set) the weights (**novelty**)
3. Use a ***double-loss ANN*** (***dl-ANN***) to learn/infer the weights for both U_x and U_y(**novelty**)

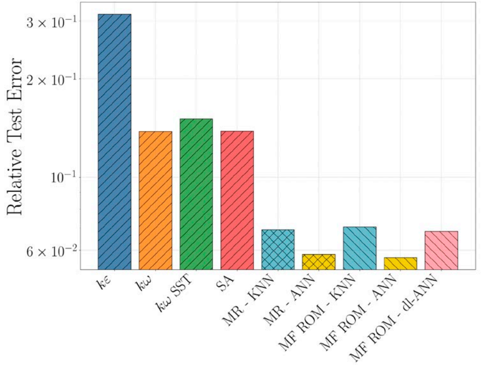


- The ANN is trained to minimize the discrepancy between the reference DNS snapshots and the aggregated solution **without knowing the expression *a priori***
- The ANN is **space-continuous**

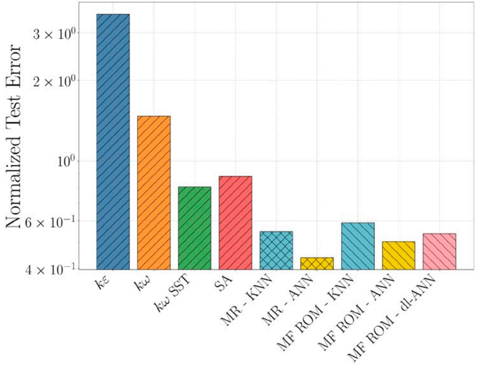
Zappi, P., Ivagnes A., Tonicello P., and Rozza G., *Aggregation pipelines using high and low-fidelity models in fluid dynamics*, in preparation.

Towards multi-fidelity: aggregation results

Aggregation results on the velocity field



Relative errors for U_x for two test parameters.



Normalized errors for U_y for two test parameters.

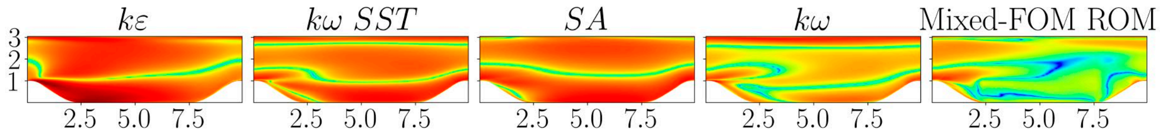
- Both aggregation pipelines provide ***higher accuracy*** than standard RANS models also in test setting
- Note that we train the aggregation ***based on only 9 DNS snapshots***
- The ANN-based aggregation provide the best results

Zappi, P., Ivagnes A., Tonicello P., and Rozza G., *Aggregation pipelines using high and low-fidelity models in fluid dynamics*, in preparation.

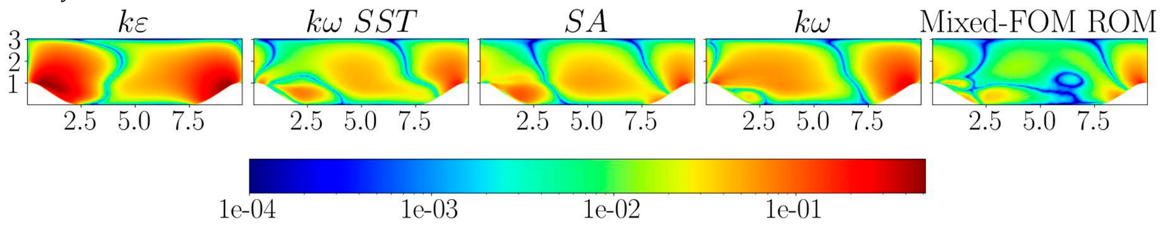
Towards multi-fidelity: aggregation results

Results in terms of absolute errors

U_x absolute errors for different individual models and for the MF-ROM - ANN aggregation.



U_y absolute errors for different individual models and for the MF-ROM - ANN aggregation.

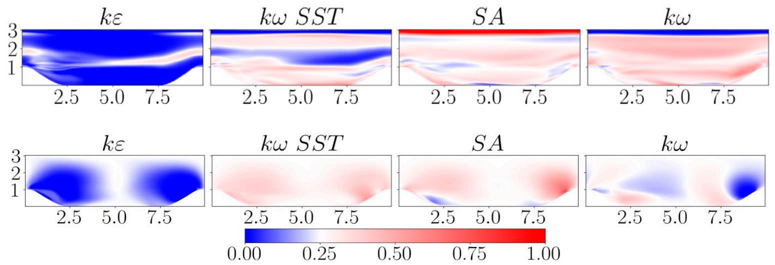


Zappi, P., Ivagnes A., Tonicello P., and Rozza G., *Aggregation pipelines using high and low-fidelity models in fluid dynamics*, in preparation.

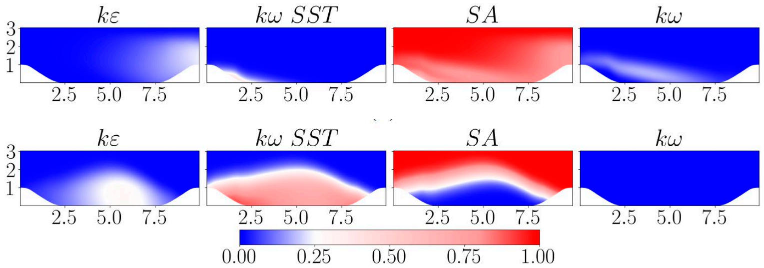
Towards multi-fidelity: aggregation results

The weights for standard aggregation and ANN-based aggregation

Weights in standard aggregation for U_x *(top) and* U_y *(bottom).*



Weights in ANN-based aggregation for U_x *(top) and* U_y *(bottom).*



- The weights of the standard aggregation are more ***physically interpretable*** and correlated to the performance of the individual models, but the ANN has the highest accuracy.

Zappi, P., Ivagnes A., Tonicello P., and Rozza G., *Aggregation pipelines using high and low-fidelity models in fluid dynamics*, in preparation.

Conclusions

- We saw different techniques to enhance the results obtained in CFD ROM frameworks with turbulence for real time computing.

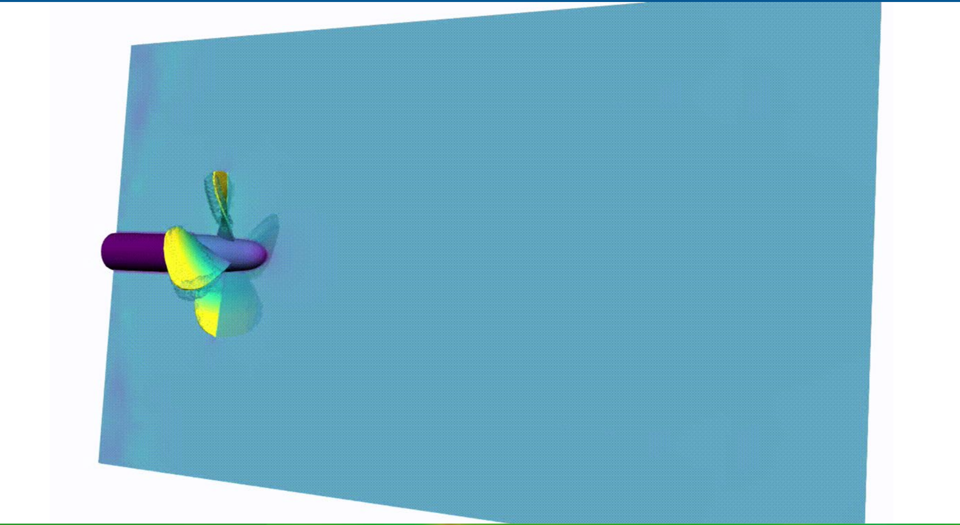
- The accuracy is improved both with scientific **machine learning** techniques (e.g. eddy viscosity coefficients) for turbulence modelling as well as closure modelling.

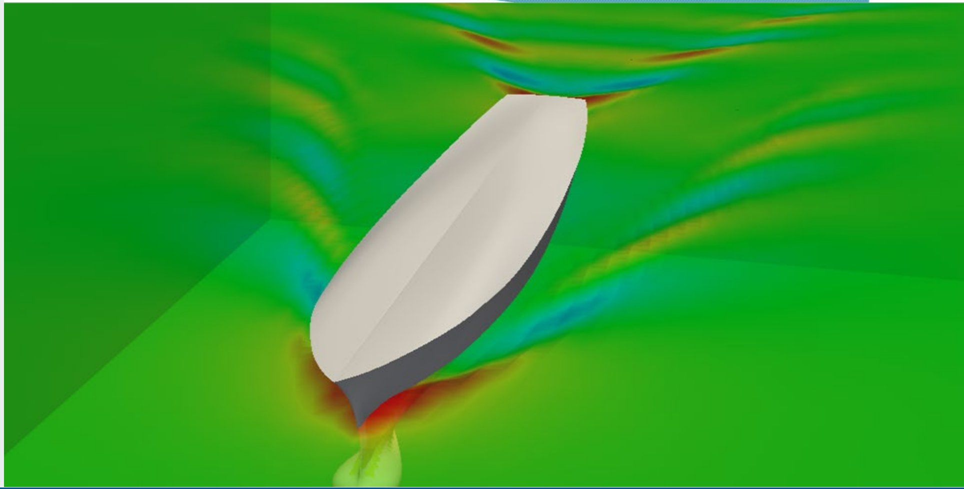
- All techniques used in non-intrusive ROMs may have bottlenecks and can be improved by **detecting the approach with the best performance** (e.g. accuracy)

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



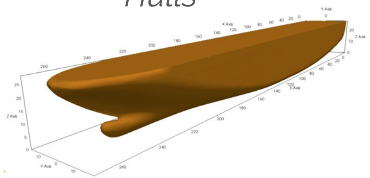


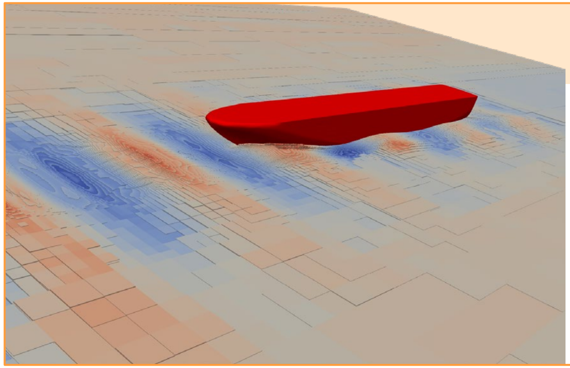
Motivation for naval design optimization

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 MARINE INNOVATION CONSULTING AND DESIGN
CETENA S.p.A.
MONTECARLOYACHTS
engys
FINCANTIERI The sea ahead

The propeller test case

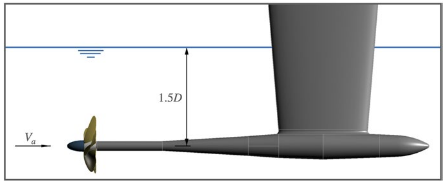
The test case: open-water tests

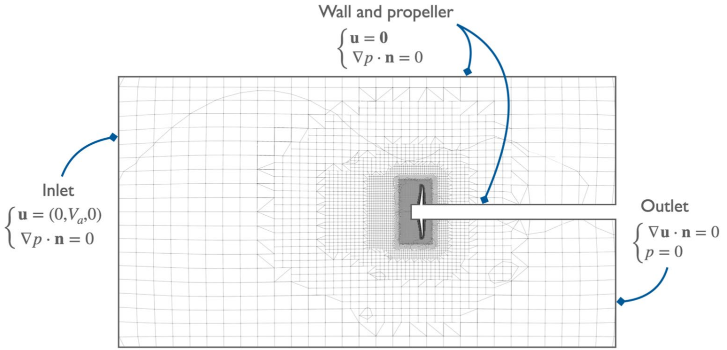
- Homogeneous inflow (velocity Va)
- Uniform and undisturbed flow conditions

The model: incompressible Navier-Stokes Equations

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

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





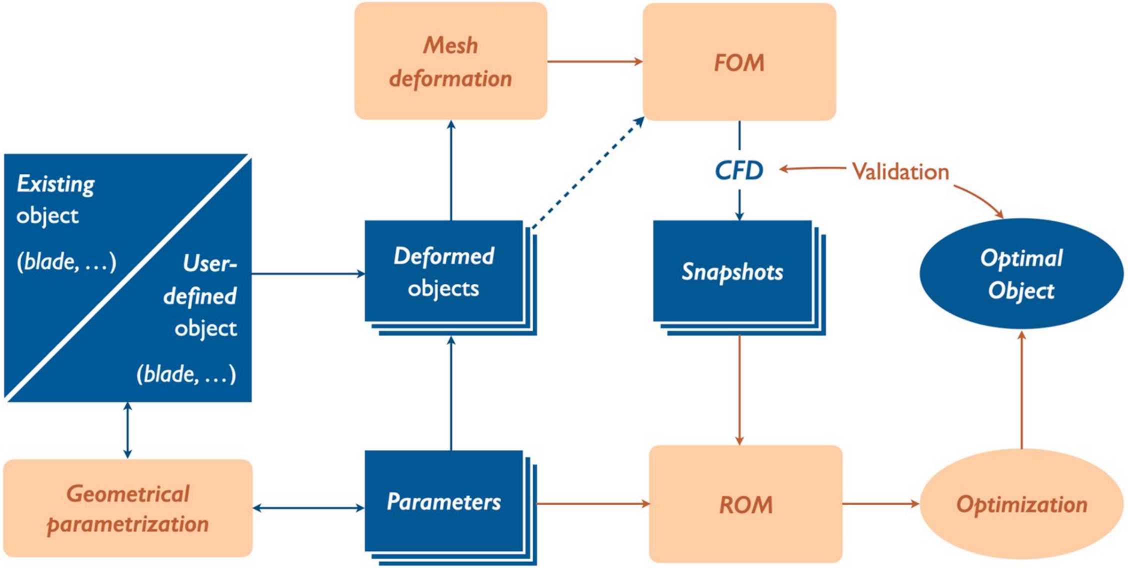
A slice of the mesh

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**

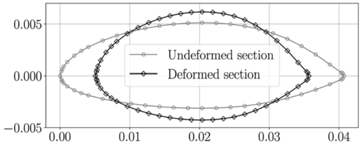


Ivagnes, Anna, Nicola Demo, and Gianluigi Rozza (2024). "A shape optimization pipeline for marine propellers by means of reduced order modeling techniques." International Journal for Numerical Methods in Engineering 125.7.

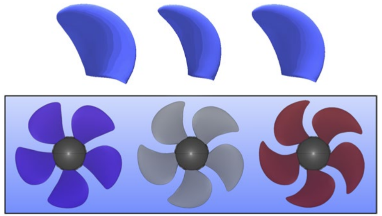
Geometric parametrization: two alternatives

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

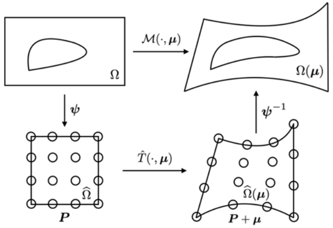


Example of blade/propeller deformation

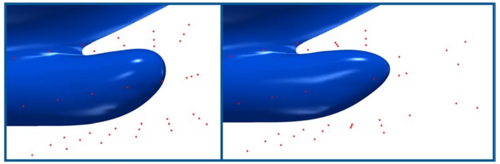
BladeX

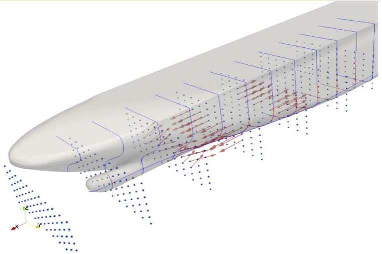
Library used

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



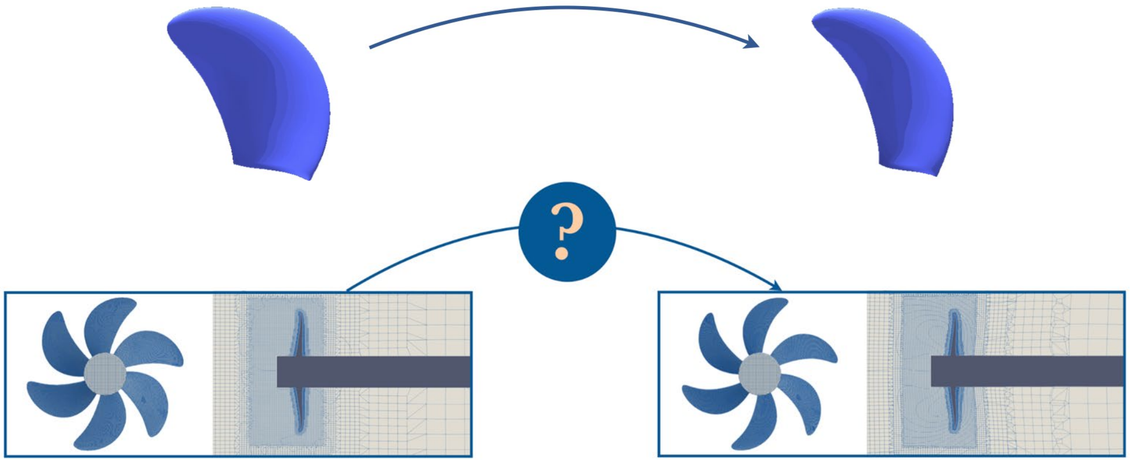
Strategy:
enclose the object in a cube, deform the cube, then back-map





Mesh deformation

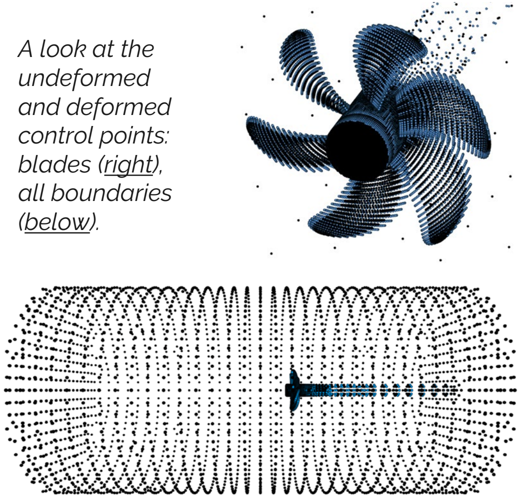
Problem: deform the mesh ***preserving the number of degrees of freedom*** in all simulations

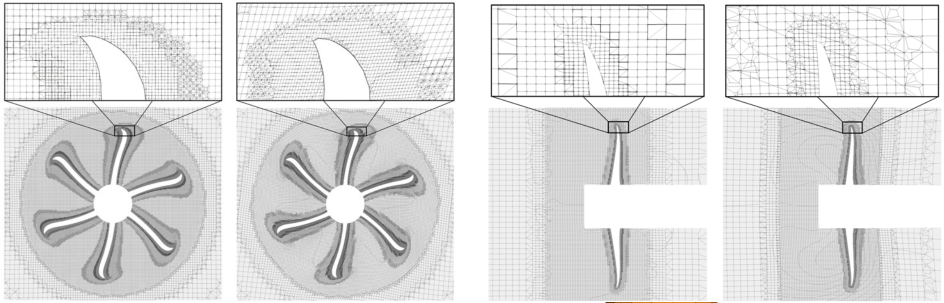


Mesh deformation

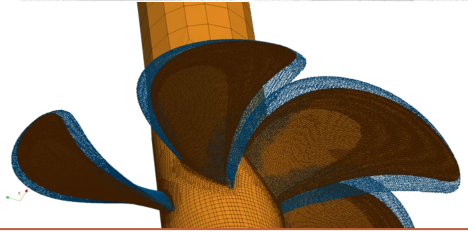
Solution: ***RBF interpolation technique***, using as ***control points*** the ***boundaries***

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

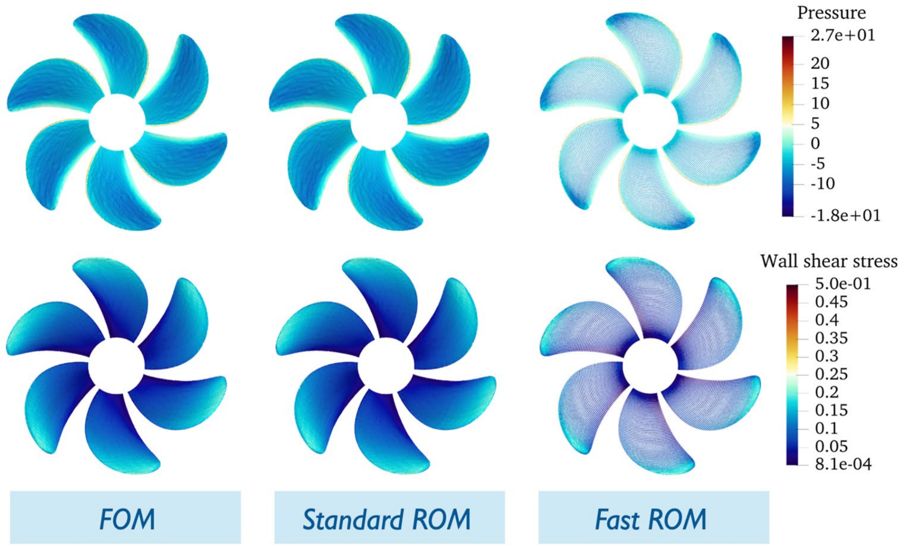
- fields evaluated at ***all blades points***
- needs to ***deform all blades points*** to compute the efficiency

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: ~ $\mathbf{10^5}$



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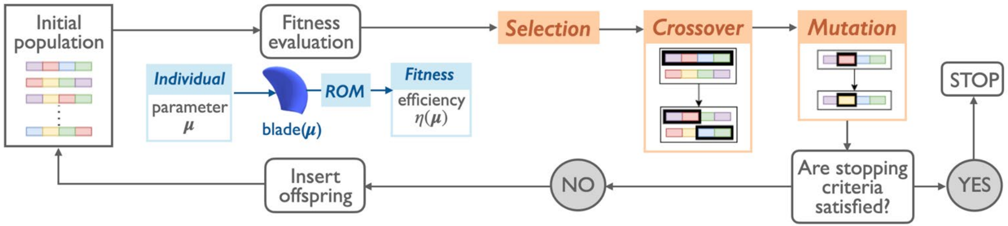
Optimization algorithm: results

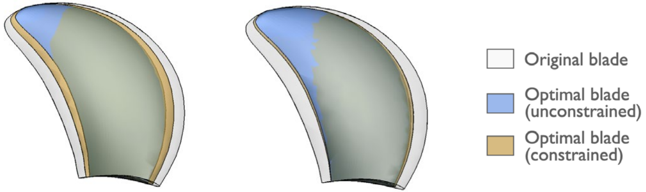
The genetic algorithm: an evolution-inspired algorithm



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)*

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