Galerkin-RB-POD Reduced Order Methods: state of the art and perspectives with focus on parametric Computational Fluid Dynamics

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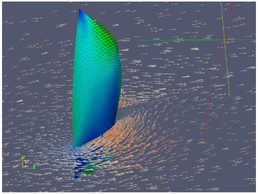
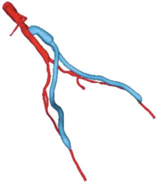
Leading Motivation: Computational Sciences challenges

- **Simulation-based science** is a quickly emerging field for mathematics and computational modelling.
- Present and future efforts: towards **multiphysics** problems, as well as systems characterized by **multiple spatial and temporal scales**.
- Growing demand of
  - **efficient computational tools** for
  - **many query** and **real time** computations,
  - **parametrized formulations**,
  - simulations of increasingly **complex systems** with uncertain scenarios,

  by **industrial and clinical** research partners.
- The 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.





Overview: our current efforts, aims and perspectives

A team developing **Advanced Reduced Order Methods** with special focus on **Computational Fluid Dynamics**

Overview: our current efforts, aims and perspectives

A team developing **Advanced Reduced Order Methods** with special focus on **Computational Fluid Dynamics**:

- to face and overcome **several limitations** of the **state of the art** for 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).

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 with ROMs (OpenFoam, Nektar, FEniCS, Libmesh)
  - ∗ **RBniCS** as educational initiative for newcomer ROM users (training).

ITHACA RBniCS

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

Reduced Order Methods: a brief historical background

An old idea...facing difficult problems

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

Pioneers of RB 1980's: Noor, Peters, Brogan, Stern, Almroth, Fink, Rheinboldt... (**Extensive Scientific Computing** was still a dream...)

New mathematical and methodological developments 2000's: Maday, Patera, Willcox, Huerta, Ito, Ravindran, Peterson, Farhat, Quarteroni, Hesthaven, Benner, Sorensen, Volkwein, Kunish, Urban, Ohlberger, Chinesta, Cueto, Ladeveze, Iollo, Perotto, Diez, Iliescu, Bergmann, Borggaard, Gunzburger ...

First mini on RB methods....ICOSAHOM Upsala 2001 and Providence 2004...organized by Maday and Patera.

Applications 2010's: several groups around the world focusing on many different aspects and applications.

Need of a better exploitation of parallel/HPC offline resources combined with reduced order methods.

We focus on RB (with POD samplings)

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:

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

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

Reduced Order Methods in a nutshell

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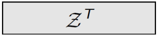
- $()_N$: reduced order method (ROM) – *the accelerator*

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

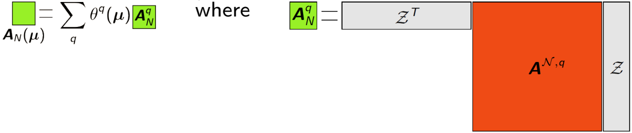


- **Online**: extremely fast (reduced order): real-time input-output evaluation

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

thanks to an efficient assembly of problem operators

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

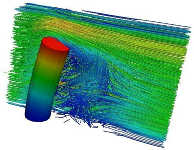


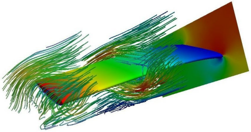
- Numerical issues: stability, error bounds, efficient parametrization, sampling, ...

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

Outline of the topics

- 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**.
- Focus of this talk: show some state of the art and perspectives in parametric flow problems treated in the reduced order context for
  - complex fluid mechanics phenomena;
  - fluid-structure interaction (FSI) reduced problems;
  - **flow control**;
  - **uncertainty quantification (UQ)**;
  - shape optimization;
  - and some perspectives and challenges.

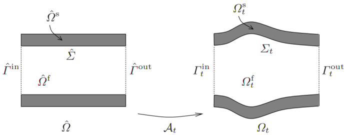




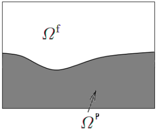
Current efforts

- Efficient management of (physical and numerical) interfaces and subdomains in a ROM setting:
  - ∗ physical interfaces:

FSI

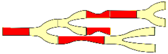


Stokes-Darcy [Martini, Haasdonk, R., 2015]

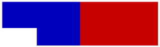


  - ∗ non-physical (computational) interfaces [Iapichino, Quarteroni, R., 2016] :

networks



domain decomposition

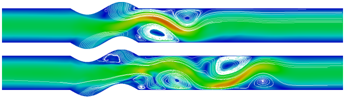


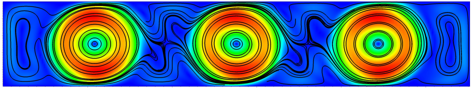
(including same physics with different mathematical models, e.g. viscous-potential coupling). [Martini, Haasdonk, R. 2017]

- Aim:
  - ∗ accurate coupling of physics,
  - ∗ keep low number of parameters,
  - ∗ dealing with moving boundaries, interfaces and domains.

#CFD

ROM and geometrical parametrization for fluid mechanics problems on moving domains Joint work with Francesco Ballarin





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

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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

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

in order to fullfil 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.)***.

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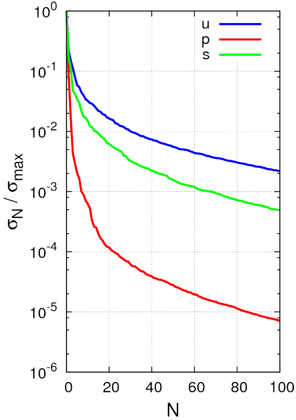
Typical reduced space dimensions and computational speedup for viscous flows



- **offline phase** in parallel on modern HPC clusters ($\mathcal{N} \approx 10^6$ dofs);
- **online phase** in serial on standard personal computer ($N \approx 10^2$ dofs);
- **considerable computational speedup**, from high-fidelity simulations that take O(day) to reduced-order ones that take O(min).

F. Ballarin, A. Manzoni, A. Quarteroni, G. Rozza. Int. J. Num. Meth. Eng., 2015.

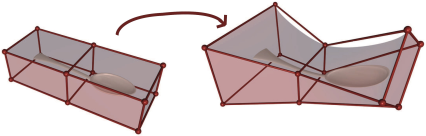
Shape parametrization for ROM

- need to combine solutions defined on different domains because (i) domain is moving and also (ii) initial configuration is parametrized,
- definition of a map

$$\Omega_o(\boldsymbol{\mu}) = \boldsymbol{T}(\Omega; \boldsymbol{\mu})$$

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].



ROM for problems on moving domains

- fluid problem in Arbitrary Lagrangian Eulerian (ALE) formulation;
- **parametrized displacement**;
- the parameter $\boldsymbol{\mu} \in \mathcal{D}$ controls (e.g.) the maximum amplitude of the deformation; $d(t)$ is a prescribed temporal profile:

$$\widetilde{\boldsymbol{\mu}}(t; \boldsymbol{\mu}) = \boldsymbol{\mu}\, d(t)$$

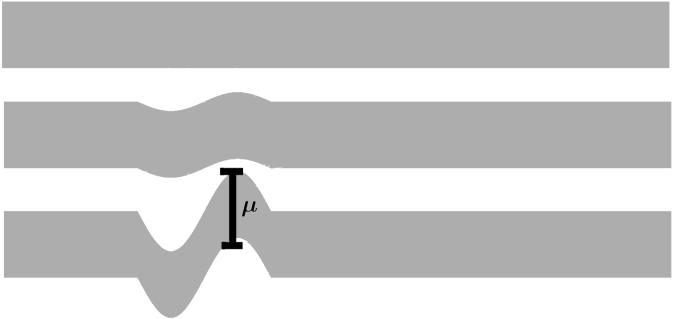
- the moving shape at time t depends both on $\boldsymbol{\mu}$ and t through $\widetilde{\boldsymbol{\mu}}(t) = \widetilde{\boldsymbol{\mu}}(t; \boldsymbol{\mu})$;
- **offline-online** decomposition of the reduced-order model is preserved/recovered **[EIM, Barrault et al., 2004]**, e.g.

$$A(t; \boldsymbol{\mu}) \overset{\text{EIM}}{\approx} \sum_{q=1}^{Q_A} \Theta_q^A(\boldsymbol{\mu}) \theta_q^A(t) A^q$$

  - the stored data structures A^q do not depend explicitly on time because the temporal dependence is stored in the multiplicative factors $\theta_q^A(t)$.

ROM for problems on moving domains: an example

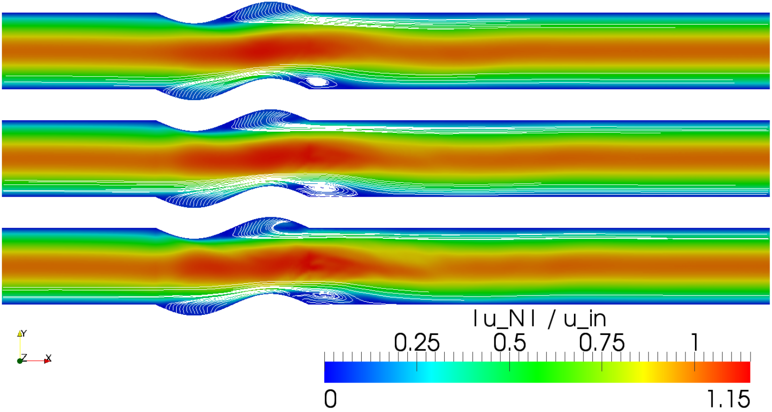
Domain: Rectangular channel of height equal to 1.
Physical parametrization: Reynolds number.
Geometrical parametrization: sinusoidal in space and in time ($T = 2\ s$) displacement of a deformable part of the domain (affine mapping). The amplitude of the peak displacement is the geometrical parameter.



Computational reduction: $N = 25$ modes capture 99.9% of the energy of NS system. Computational savings of $\approx 95\%$ (online POD–Galerkin vs FEM). Offline stage for 60 random snapshots $\times$ 100 timesteps: 1.5 days.

ROM for problems on moving domains: results

$\mu = 0.5, t = 0.75\ s$. From top to bottom: $Re = 400, 600, 800$:

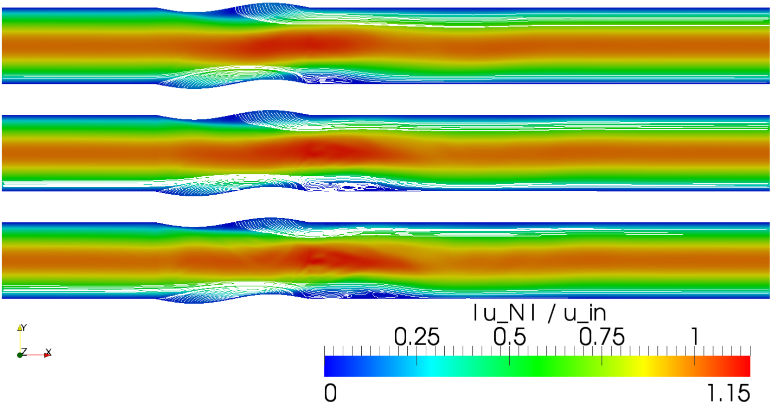


Small displacement: one small vortex propagates downstream...

F. Ballarin, G. Rozza, IJNMF, 2016.

ROM for problems on moving domains: results

$\mu = 0.5, t = 0.9\ s$. From top to bottom: $Re = 400, 600, 800$:



Small displacement: ... and is rapidly dissipated.

F. Ballarin, G. Rozza, IJNMF, 2016.

ROM for problems on moving domains: results

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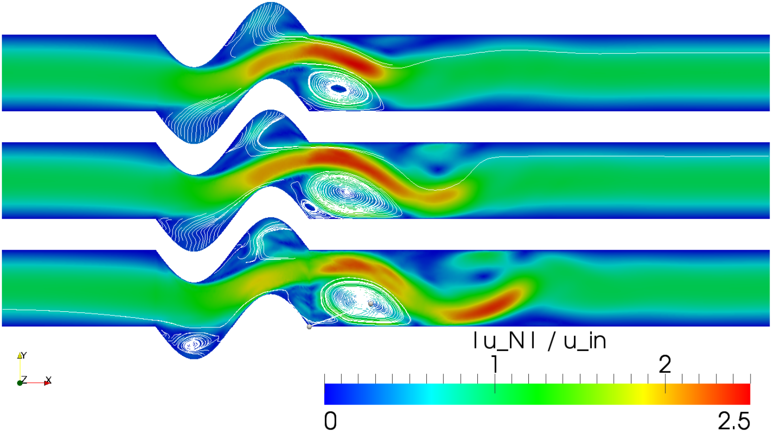
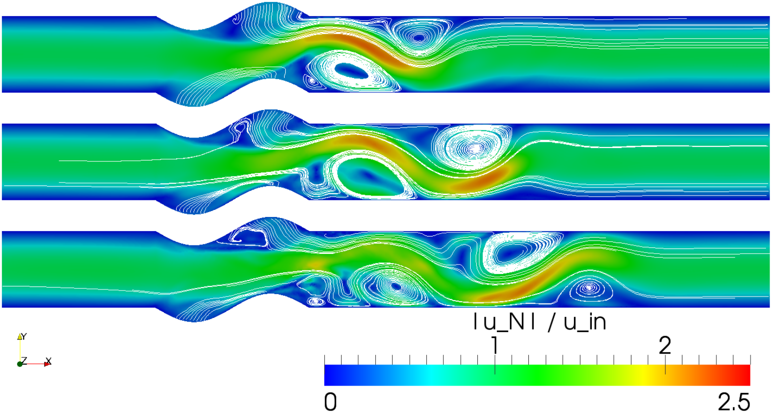


Large displacement: a bigger vortex propagates downstream, together with a jet at higher velocity...

F. Ballarin, G. Rozza, IJNMF, 2016.

ROM for problems on moving domains: results

$\mu = 1.5, t = 0.9\ s$. From top to bottom: $Re = 400, 600, 800$:



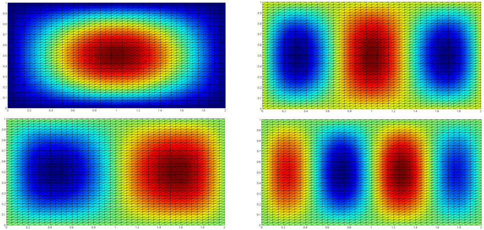
Large displacement: ... and other vortices may appear, depending on the Reynolds number.

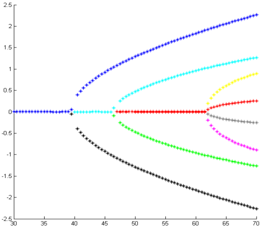
F. Ballarin, G. Rozza, IJNMF, 2016.

Some ROM challenges

Bifurcation and stability analysis of parametrized (fluid dynamics and mechanics) problems by ROM

- **Stability studies** in nonlinear problems are very expensive.
- Understand and detect complex phenomena, such as **bifurcations**, leading to loss of uniqueness of the solution also at the reduced order level.
- Efficient reduced numerical techniques to detect **steady and Hopf bifurcations and branching** (continuation, eigenvalues analysis, efficient sampling, error bounds).
- Efficient sampling / A posteriori error estimation.
- **Computational mechanics problems** to study the deformation of a plate under compression and the bifurcations of the Von Kaŕmań model through the linearized eigenvalues problem.



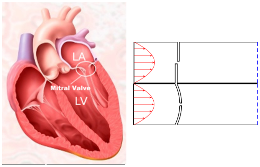


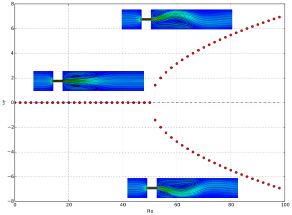
- Towards multi-physics studies.

in collaboration with Giuseppe Pitton (SISSA), Annalisa Quaini (Houston), Federico Pichi (SISSA), Anthony Patera (MIT), Martin Hess (SISSA), Max Gunzburger and Alessandro Alla (Florida State).

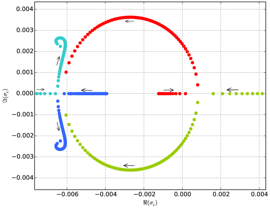
Some ROM challenges in CFD

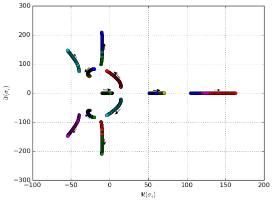
- **Complex CFD problems** in 3D setting characterized by bifurcations, e.g. Coanda effect in **mitral valves**, influence of more complex geometries and multiphysics on bifurcations and stability.





Investigations on bifurcations and loss of uniqueness of the solution require ROM for parametrized eigenvalue analysis. [Pitton, R., 2017, JSC.; Pitton, Quaini, R., 2017, JCP.]

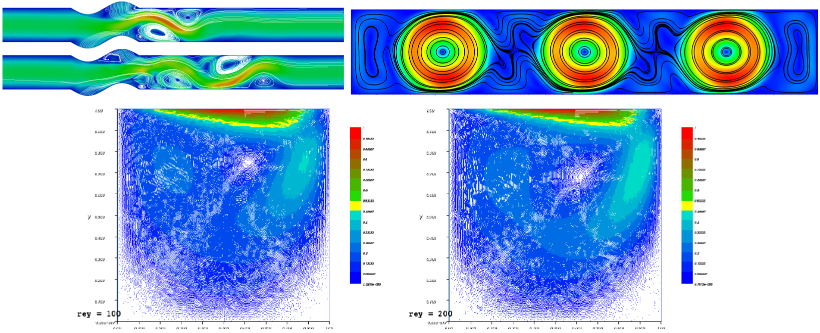




Some ROM challenges in CFD

Higher Reynolds parametrized flows in ROM

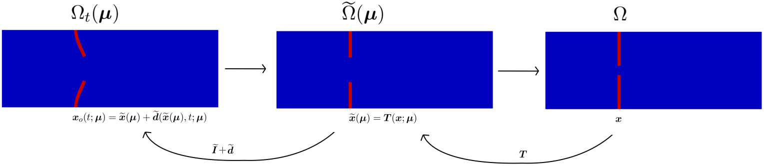
- Low and moderate Reynolds numbers for ROM of parametrized viscous flows. We need to **increase Reynolds number**.
- Offline–Online **stabilization techniques** for parametrized flows (geometry, physics) derived from streamline upwind Petrov-Galerkin (SUPG), . . .
- A ROM **variational multiscale** approach in parametrized context to be properly developed, towards turbulence modelling, Smagorinski turbolent model [T. Chacón Rebollo, E. Delgado, et al.].
- Important expectations and needs dealing with **industrial and cardiovascular flows**.



in collaboration with Shafqat Ali, Giovanni Stabile, Giacomo Zuccarino (SISSA).

#FSI

Monolithic ROMs for FSI problems
Joint work with Francesco Ballarin.



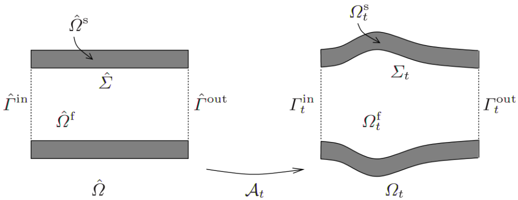
Formulation of FSI problems

- 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

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



Previous reduced order approaches to FSI problems

- [Lassila *et al.*, 2012] and [Lassila *et al.*, 2013] (1D structural model, parametric interface coupling to RB fluid problem Stokes/Navier-Stokes, respectively, axialsymmetry),
- [Colciago, Ph.D. thesis, 2014] (fixed domain and thin-walled structure, RB for fluid problem with generalized Robin boundary conditions),
- [Bertagna, Veneziani, 2014] (1D structural model, POD–Galerkin),
- [Forti, Rozza, 2014] (efficient geometrical parametrization of interfaces, modal greedy),
- [Lieu *et al.*, 2006], ..., [Amsallem *et al.*, 2013], [Amsallem *et al.*, 2015] (aeroelasticity),

Our approach:

- no simplifications for structural model,
- POD–Galerkin method for **global** variables $\boldsymbol{u}, p, \boldsymbol{d}$ (monolithic approach), time dependent,
- capability to parametrize the initial configuration (geometry).

Reduced order monolithic formulation of FSI problems

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

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

$$\begin{aligned} F^{\mathcal{N}}(\boldsymbol{u}_f^{\mathcal{N}}(\boldsymbol{\mu}), p^{\mathcal{N}}(\boldsymbol{\mu}), \boldsymbol{d}_f^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{d}_s^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) &= 0 \quad \text{Fluid} \\ S^{\mathcal{N}}(\boldsymbol{u}_s^{\mathcal{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) &= 0 \quad \text{Structure} \\ I^{\mathcal{N}}(\boldsymbol{d}_f^{\mathcal{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathcal{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) &= 0 \quad \text{Interface} \\ \text{coupling conditions} & \end{aligned}$$

OFFLINE – Space construction and matrices assembling

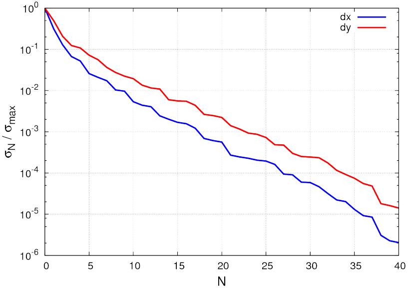
- Space construction by **Proper Orthogonal Decomposition** for **global** variables.
- Additional computations related to inf-sup stabilization procedure by means of supremizer enrichment $\rightarrow$ accurate pressure recovery for balance of normal forces. [Ballarin et al., 2015], [Rozza *et al.*,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

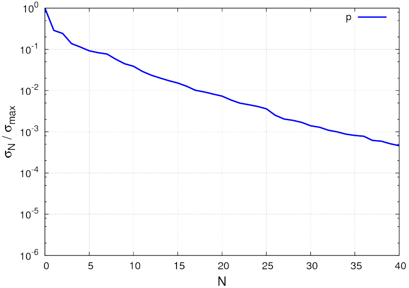
ONLINE – Galerkin projection over the enriched space

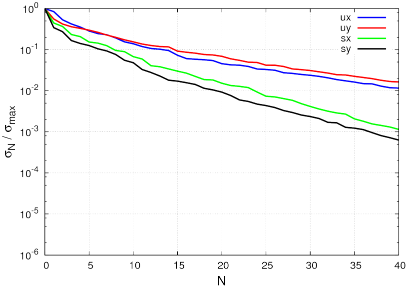
For $\boldsymbol{\mu} \in \mathcal{D}$, solve $\mathbf{N} \ll \mathcal{N}$

$$\begin{aligned} F^{\mathbf{N}}(\boldsymbol{u}_f^{\mathbf{N}}(\boldsymbol{\mu}), p^{\mathbf{N}}(\boldsymbol{\mu}), \boldsymbol{d}_f^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{d}_s^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) &= 0 \quad \textbf{Reduced} \text{ fluid} \\ S^{\mathbf{N}}(\boldsymbol{u}_s^{\mathbf{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) &= 0 \quad \textbf{Reduced} \text{ structure} \\ I^{\mathbf{N}}(\boldsymbol{d}_f^{\mathbf{N}}(\boldsymbol{\mu}), \boldsymbol{d}_s^{\mathbf{N}}(\boldsymbol{\mu}); \boldsymbol{\mu}) &= 0 \quad \textbf{Reduced} \text{ interface} \\ \text{coupling conditions} & \end{aligned}$$

Reduced order monolithic formulation of FSI problems: results (1)







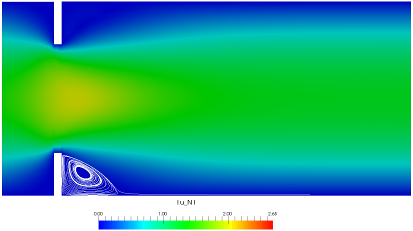
POD singular values for (global) displacement, pressure, velocity and supremizers.

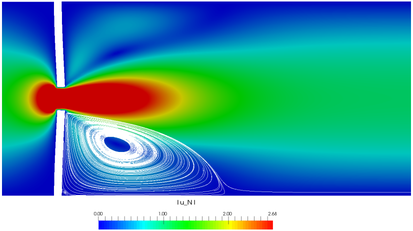
Fastest decay: displacement (top left).

Slower decay for velocity and supremizers modes (bottom left).

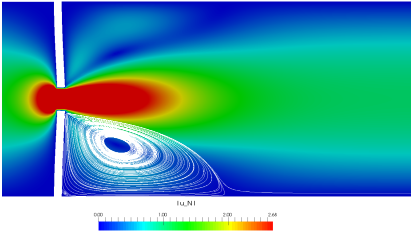
Ongoing applications to cardiovascular modelling

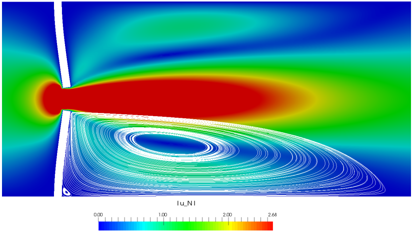
Increase leaflet length: *(same inlet velocity)*





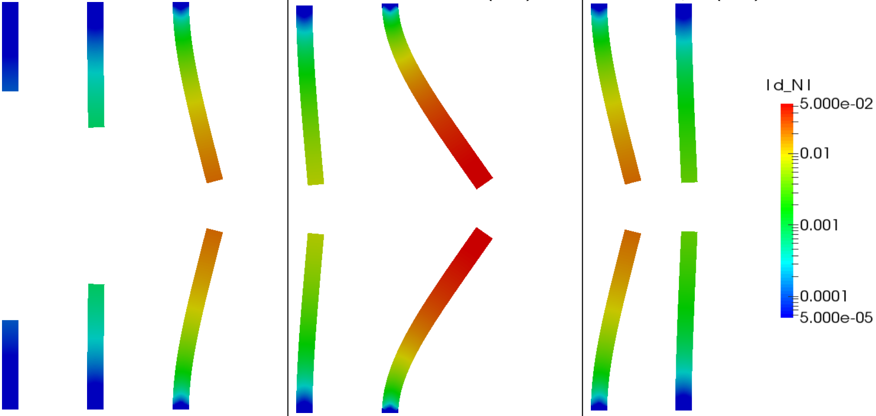
Increase inlet velocity: *(same leaflet length)*





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. IJNMF, 2016.*
- *F. Ballarin, G. Rozza, Y. Maday. Reduced-order semi-implicit schemes for fluid-structure interaction problems. MS&A, vol. 17*

Some ROM challenges in CFD

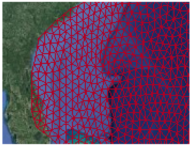
Reduced order models for inverse problems, flow control, shape optimization, and uncertainty quantification

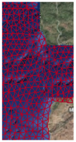
- Importance of optimal control in a **parametrized setting**, as well as **(shape) optimization** and more general **inverse problems**.
- After simulation (1990s), control and optimization (2000s), the new paradigm is **reduction for real-time control and optimization** (2010s), in view of more and more complex approaches (multiphysics, multi-phase, domain decomposition, interfaces).
- **Uncertainty Quantification** (UQ) is a growing topic in applied mathematics with several potential applications in **bridging models and reality by data**.
- Mathematical models need quantification of uncertainty to improve their efficacy and synthesis, and their **applicability scenarios**.
- **Computational Reduction strategies** are important to deal with high dimensional problems in terms of random parameters as well as for **data assimilation, parameter estimation, risk analysis (SIAM JUQ Review 2017 - Chen, Quarteroni, Rozza**.
- **Hierarchical Model Reduction.**

Collaboration: Peng Chen (ETHZ, Austin), Davide Torlo (Zurich), Luca Venturi (Courant Inst.), Matteo Zancanaro, Maria Strazzullo, Zakia Zainib, Monica Nonino (SISSA), Alfio Quarteroni (EPFL), Giulia Meglioli, Simona Perotto (POLIMI).

#CFD

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





Model Reduction for Parametrized Optimal Control Problems in offline–online computing

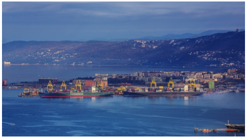
- Reduced order models have been applied to parametrized linear-quadratic advection-diffusion optimal control problems in different contexts: [Dedé, 2010], [Tonn *et al.*, 2010], [Grepl, Kärcher, 2011] [Quarteroni et al., 2007];
- several recent contributions to build a reduced order framework to handle general control functions, i.e. **infinite dimensional** distributed and/or boundary **control** functions, error bounds, more complex 2D-3D geom. parametrizations [Rozza et al., 2012],[Negri et al., 2013],[Kärcher, Grepl, 2014], [Kärcher, Grepl, Veroy, 2014], [Negri et al., 2015] and parametrized control of stochastic PDEs [Chen et al., 2013], [Chen et al., 2015].

Collaborations

The numerical results have been reached in collaboration with Prof. R. Mosetti (National Institute of Oceanography and Applied Geophysics, OGS, Trieste, Italy).

Why do we use Reduced Order Methods (ROM) for parameterized Optimal Flow Control Problems (OFCP(μ)) in environmental sciences?

1. problems dealing with environmental marine sciences must be run many times for different values of $\boldsymbol{\mu}$. The developed framework is suited for **data assimilation**, **inverse problems**, as well as **uncertainty quantification** and **parameter estimation problems**. A **fast** and **reliable** tool is needed
2. ROMs allow to study several configuration in order to **manage rapidly** and **efficiently** different (potentially dangerous) **situations**.



The abstract optimization problem

Notation: $y, z \in Y$ state space $\quad u, v \in U$ control space

$p, q \in Q \,(\equiv Y)$ adjoint space $\quad \mathcal{Z}$ observation space s.t. $Y \subset \mathcal{Z}$

Parametrized optimal control problem: given $\boldsymbol{\mu} \in \mathcal{D}$

$$\text{minimize} \quad J(y, u; \boldsymbol{\mu}) = \frac{1}{2}\mathbf{m}(y - y_d(\boldsymbol{\mu}), y - y_d(\boldsymbol{\mu}); \boldsymbol{\mu}) + \frac{\alpha}{2}\mathbf{n}(u, u; \boldsymbol{\mu})$$

$$\text{s.t.} \quad \mathbf{a}(y, q; \boldsymbol{\mu}) = \mathbf{c}(u, q; \boldsymbol{\mu}) + \langle G(\boldsymbol{\mu}), q \rangle \qquad \forall q \in Q.$$

Compact abstract form/notation

given $\boldsymbol{\mu} \in \mathcal{D}$, find $\mathrm{U}(\boldsymbol{\mu}) \in \mathcal{X}$ s.t:

$$\mathrm{B}(\mathrm{U}(\boldsymbol{\mu}), \mathrm{W}; \boldsymbol{\mu}) = \mathrm{F}(\mathrm{W}; \boldsymbol{\mu}) \quad \forall\, \mathrm{W} \in \mathcal{X}.$$

$$\mathcal{X} = Y \times U \times Q,$$
$$\mathrm{U} = (y, u, p), \quad \mathrm{W} = (z, v, q)$$

- at this point we may apply the Galerkin-FE approximation ("truth" approx.)

ROMs for Environmental OFCP($\boldsymbol{\mu}$)s

We have applied ROMs reduction methods to optimal control in environmental marine problems.
We focused on the monitoring of the Gulf of Trieste, Italy.

1. Pollutant control on the Gulf of Trieste: **why?**
   - forecasting,
   - data assimilation, parameter estimation, uncertainty quantification.
   - ecological and touristic interests,
   - geographical interest.

Pollutant Control on Gulf of Trieste

Problem formulation
[$y \in H^1_{\Gamma_D}(\Omega), u \in \mathbb{R}$,
$y_d \in \mathbb{R}$ (safeguard threshold)]:

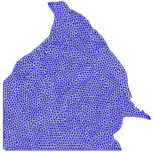
Weak formulation

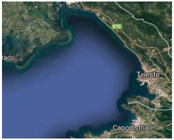
Minimise with respect to
$(y(\boldsymbol{\mu}), u(\boldsymbol{\mu})) \in Y \times U$

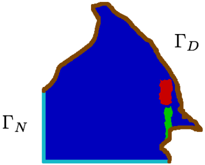
$$J(y,u) = \frac{1}{2}\int_{\Omega_{OBS}} (y(\boldsymbol{\mu}) - y_d)^2 \, d\Omega_{OBS}$$

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, Italy).

Weak Formulation of the Problem

- $a : Y \times Q \to \mathbb{R} : \; a(y, q, \boldsymbol{\mu}) = \displaystyle\int_\Omega (\nu(\boldsymbol{\mu}) \nabla y \cdot \nabla q + \boldsymbol{\beta}(\boldsymbol{\mu}) \cdot \nabla y q) \, d\Omega,$
- $c : U \times Q \to \mathbb{R} :$
  $c(u, q) = L \, u \displaystyle\int_{\Omega_u} q \, d\Omega_u,$ $[L = 10^3 \to$ non-dimensional system$]$

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

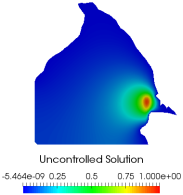
$\nu(\boldsymbol{\mu}) \equiv \mu_1$ is the diffusivity parameter,

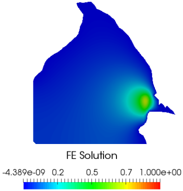
$\boldsymbol{\beta}(\boldsymbol{\mu}) = [\beta_1(\mu_2), \beta_2(\mu_3)]$ is the transport field,

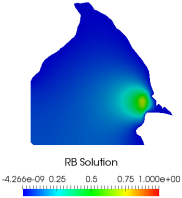
Table: **Control and cost functional value for several parameters**

	$\boldsymbol{\mu}$	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)	$8.0800 \cdot 10^{-1}$	$5.3417 \cdot 10^{-5}$

Numerical Results: FE vs POD Solutions (Bora)







Parameter: $\boldsymbol{\mu} = (1, -1, 1)$.

Sampling distribution for POD: Uniform.

Training set dimension: 100.

Time of resolution: $t_{\mathcal{N}} = 2.79s$ and $t_N = 2.41 \cdot 10^{-2}s$.

Dimensions: $\mathcal{N} = 5639$ and $N = 20$.

[Strazzullo *et al.*, Model Reduction for Parametrized Optimal Control Problems in Environmental Marine Sciences and Engeneering, SIAM SISC, submitted, 2017]

Numerical Results: FE – POD Errors

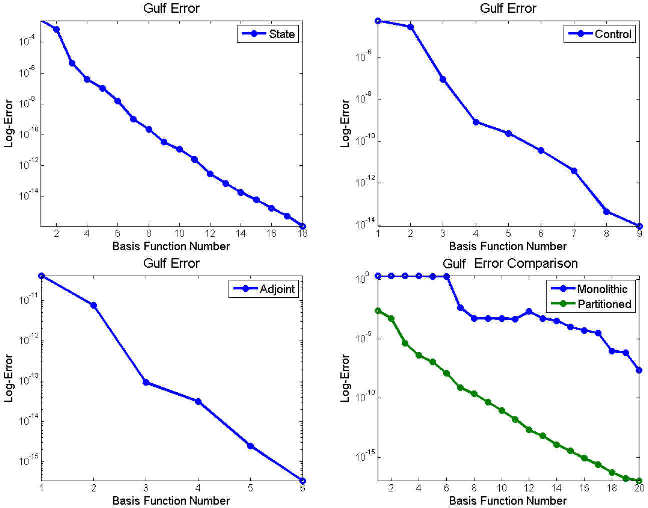
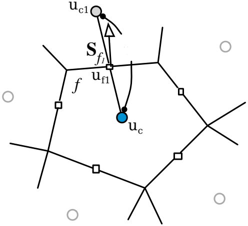


Figure: Bora Errors. *Bottom right*: monolithic (one POD for $U(\boldsymbol{\mu}) = (y(\boldsymbol{\mu}), u(\boldsymbol{\mu}), q(\boldsymbol{\mu}))$) and partitioned (different POD reductions for state, control and adjoint variables) error comparison. [partitioned much better results $\rightarrow$ approach chosen for the next application].

Industrial #CFD

ROM for Finite Volume Approximations and Industrial Flows (Higher Reynolds Numbers) Joint work with Giovanni Stabile



Overview of the physical problems of interest

The interest is in **viscous steady and unsteady parametrized incompressible/compressible flows** with **moderate-high Reynolds number**

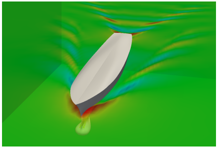


Figure: Naval Eng.

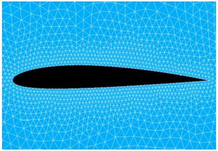


Figure: Aeronautics

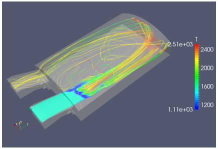


Figure: Industrial App.

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 Higher Reynolds Number?

- Many **industrial applications** require turbulent flows.
- At full order level, for what concern **finite volumes**, **many turbulent models** have been developed during the years.
- For **finite elements** there are several stabilization techiniques that could be exploited.

Two different strategies are under investigation in our group:

Finite Volumes	Finite Elements
• Developed turbulent ROMs (higher Reynolds number) starting from $k-\omega$ RANS and one-eq. LES full order models. Saddam Hijazi (SISSA)	• Turbulent ROMs (moderate Reynolds number) starting from Residual Based-VMS stabilization techniques full order models. Giacomo Zuccarino (SISSA).

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?

- ☺ It became the standard for real world applications in several engineering fields (Aeronautics, Industrial flows, Automotive, Naval Engineering)
- ☺ 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.
- ☹ More difficulties into the affine decomposition of the differential operators.
- ☹ The ROM methodology, mainly developed for FEM solvers, needs to be adapted.
- ☹ The geometrical parametrization includes many more difficulties respect to a finite element setting.

Issues in FV and Reduced Order Modelling

To export the ROM methodology, mainly developed for finite element solvers, into a **Finite Volume setting** several issues need to be tackled.

- Adapt ROM methods to **finite volume approximations** [Haasdonk and Ohlberger (2008)].
- Implement efficient **POD-Galerkin** strategies [Lorenzi et al (2016)].
- **Geom. Parametrization** for non-linear problems [Drohmann et al (2009)].
- **Stabilization** issues for **incompressible** flows [Rozza et al., Noack, Akhtar..].
- **Stabilization for compressible flows** and **long time** intervals [Carlberg et al (2017) , Balajewicz et al. (2016))].
- Develop ROMs **beyond** the **laminar assumption**.
- G. Stabile, S. Hijazi, A. Mola, S. Lorenzi, and G. Rozza. Advances in Reduced order modelling for CFD: vortex shedding around a circular cylinder using a POD-Galerkin method. In Press, 2017 CAIM

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Generation of the POD spaces

There are several techniques to obtain the hierarchical reduced order spaces later used for the Galerkin projection:

- **POD**
- RB with greedy sampling algorithm

The reduced order space V_u and Q_p are constructed using a **SVD** on the snapshots matrices of **velocity** and **pressure**:

$$\mathcal{U}' = [\boldsymbol{u}'(t_1), \boldsymbol{u}'(t_2), ..., \boldsymbol{u}'(t_n)] \text{ with } \boldsymbol{u}'(t) = \boldsymbol{u}(t) - \overline{\boldsymbol{u}} \quad (1)$$

$$\mathcal{P} = [\boldsymbol{p}(t_1), \boldsymbol{p}(t_2), ..., \boldsymbol{p}(t_n)] \quad (2)$$

$$\mathcal{U}' = \mathcal{W}^u \Sigma^u \mathcal{V}^{uT}, \quad \mathcal{W}^u = [\phi_1, \phi_2, ..., \phi_n], \quad \Sigma^u_{ii} = \lambda^u_i \quad (3)$$

$$\mathcal{P} = \mathcal{W}^p \Sigma^p \mathcal{V}^{pT}, \quad \mathcal{W}^p = [\chi_1, \chi_2, ..., \chi_n], \quad \Sigma^p_{ii} = \lambda^p_i \quad (4)$$

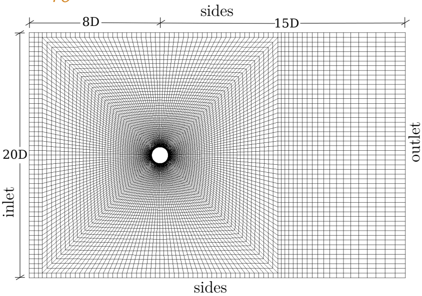
We can **truncate** the dimension of the reduced basis space looking at the eigenvalues and we can finally construct the reduced basis spaces for the **Galerkin projection**:

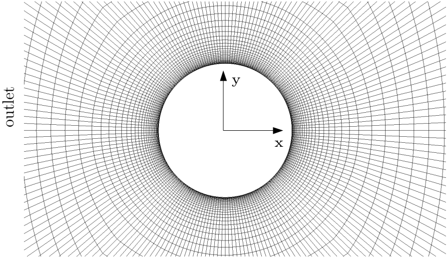
$$\mathbb{V}_{N_u} = \text{span}(\phi_1, \phi_2, ..., \phi_{N_u}) \qquad \mathbb{Q}_{N_p} = \text{span}(\chi_1, \chi_2, ..., \chi_{N_p})$$

ROM for Finite Volume Approximations and Industrial Flows

A first benchmark to understand the best strategy for **pressure reconstruction with ROM-FV.** A **supremizer stabilization** technique and a **pressure Poisson equation** strategies have been compared. The mesh counts **13296** hexahedral elements. The full order model is solved using OpenFOAM

$T_{CPU_{FO}} = 1483\mathbf{s} \approx 25\mathbf{min}$

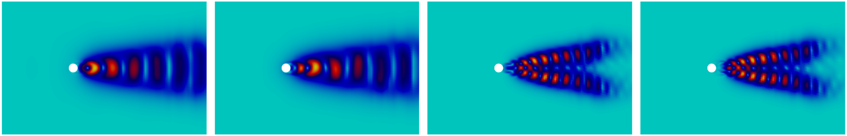




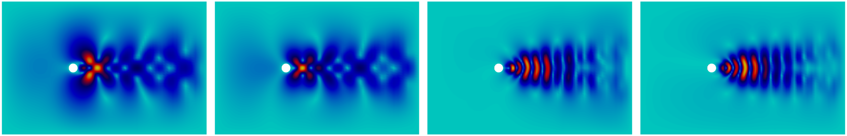
	inlet	outlet	cylinder	sides
$\boldsymbol{u}$	$\boldsymbol{u_{in}} = [u_{x_{in}}, 0]$	$\nabla \boldsymbol{u} \cdot \boldsymbol{n} = \boldsymbol{0}$	$\boldsymbol{u} = \boldsymbol{0}$	$\boldsymbol{u} = 0$
p	$\nabla p \cdot \boldsymbol{n} = 0$	$p = 0$	$\nabla p \cdot \boldsymbol{n} = 0$	$\nabla p \cdot \boldsymbol{n} = 0$

ROM for Finite Volume Approximations and Industrial Flows

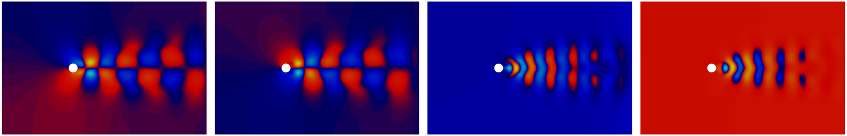
First four modes of POD velocity space



First four modes of the POD supremizer space



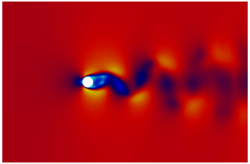
First four modes of the POD pressure space



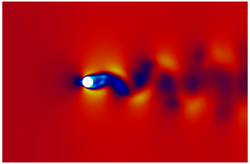
A Numerical Example

Velocity Reconstruction

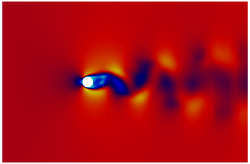
FO, $t = 1\Delta t$



PPE, $t = 1\Delta t$

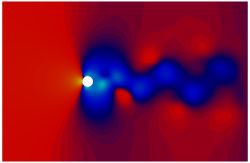


SUP, $t = 1\Delta t$

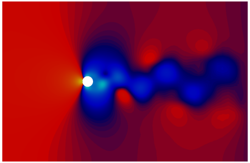


Pressure Reconstruction

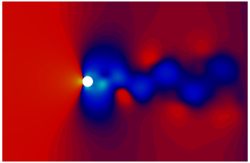
FO, $t = 1\Delta t$



PPE, $t = 1\Delta t$



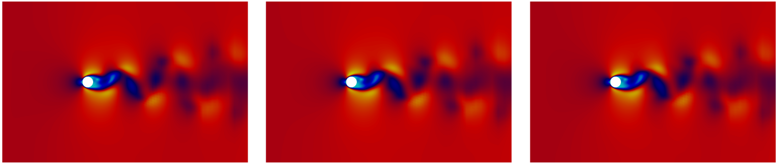
SUP, $t = 1\Delta t$



A Numerical Example

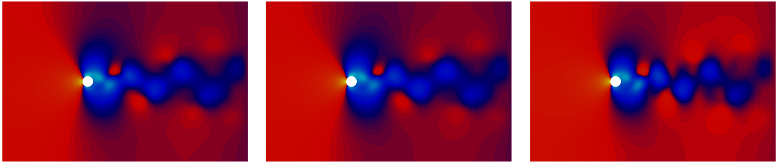
Velocity Reconstruction

FO, $t = 20\Delta t$ PPE, $t = 20\Delta t$ SUP, $t = 20\Delta t$



Pressure Reconstruction

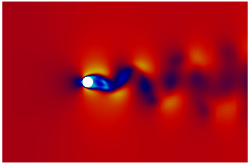
FO, $t = 20\Delta t$ PPE, $t = 20\Delta t$ SUP, $t = 20\Delta t$



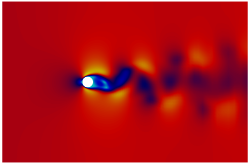
A Numerical Example

Velocity Reconstruction

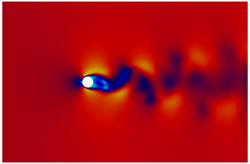
FO, $t = 40\Delta t$



PPE, $t = 40\Delta t$

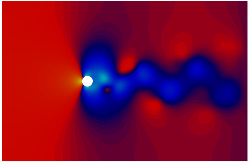


SUP, $t = 40\Delta t$

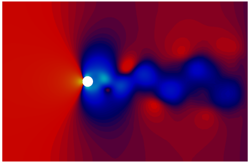


Pressure Reconstruction

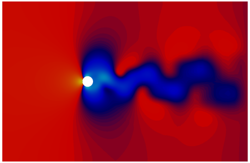
FO, $t = 40\Delta t$



PPE, $t = 40\Delta t$



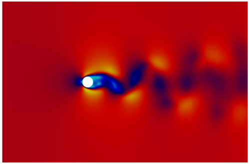
SUP, $t = 40\Delta t$



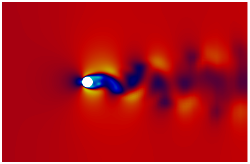
A Numerical Example

Velocity Reconstruction

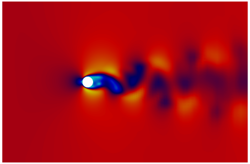
FO, $t = 60\Delta t$



PPE, $t = 60\Delta t$

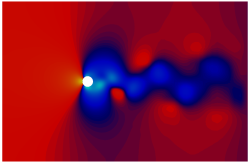


SUP, $t = 60\Delta t$

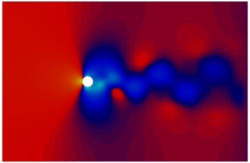


Pressure Reconstruction

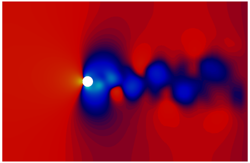
FO, $t = 60\Delta t$



PPE, $t = 60\Delta t$



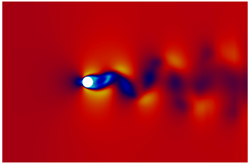
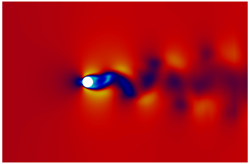
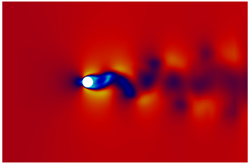
SUP, $t = 60\Delta t$



A Numerical Example

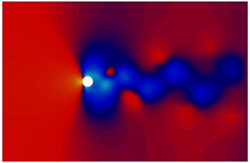
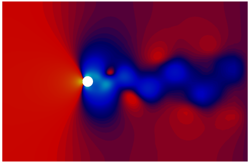
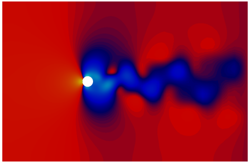
Velocity Reconstruction

FO, $t = 80\Delta t$ | PPE, $t = 80\Delta t$ | SUP, $t = 80\Delta t$

Pressure Reconstruction

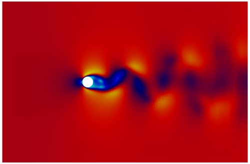
FO, $t = 80\Delta t$ | PPE, $t = 80\Delta t$ | SUP, $t = 80\Delta t$

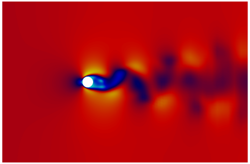
A Numerical Example

Velocity Reconstruction

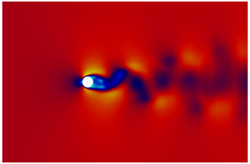
FO, $t = 100\Delta t$



PPE, $t = 100\Delta t$

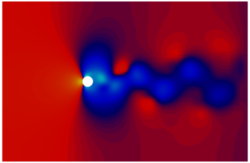


SUP, $t = 100\Delta t$

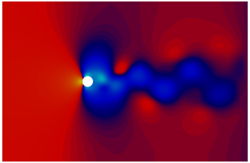


Pressure Reconstruction

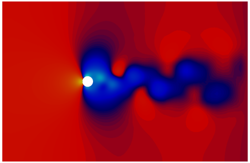
FO, $t = 100\Delta t$



PPE, $t = 100\Delta t$



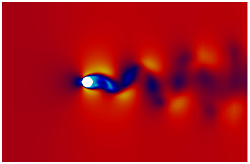
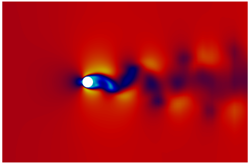
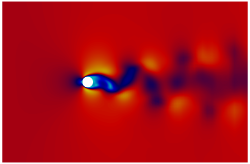
SUP, $t = 100\Delta t$



A Numerical Example

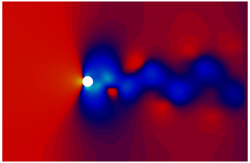
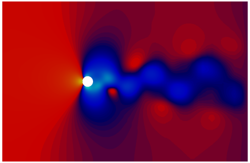
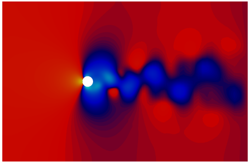
Velocity Reconstruction

FO, $t = 120\Delta t$ | PPE, $t = 120\Delta t$ | SUP, $t = 120\Delta t$

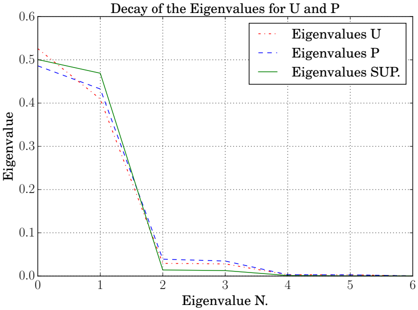




Pressure Reconstruction

FO, $t = 120\Delta t$ | PPE, $t = 120\Delta t$ | SUP, $t = 120\Delta t$

ROM for Finite Volume Approximations and Industrial Flows



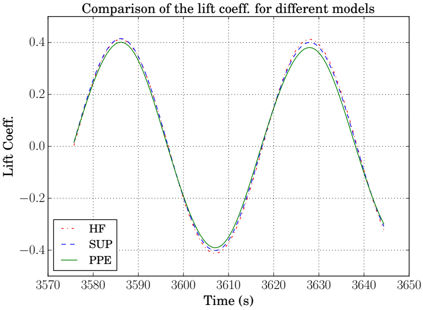


Table: Comparison of the different methods

	ε_U	ε_p	comp. time	SpeedUp
without stab $(10\phi, 5\chi)$	NaN	NaN	NaN	Nan
without stab (10ϕ)	1.25%	-	2.16 s	823
with sup. $(10\phi, 5\chi, 5\boldsymbol{sup})$	1.95%	0.67%	4.83 s	68
with PPE $(10\phi, 5\chi)$	1.25%	0.51%	3.525 s	506

$$\varepsilon_U = \frac{1}{N_t}\sum_{i=1}^{N_t} \|u_{FO}(i) - u_{ROM}(i)\|_{L^2(\Omega)} \qquad \varepsilon_p = \frac{1}{N_t}\sum_{i=1}^{N_t} \|p_{FO}(i) - p_{ROM}(i)\|_{L^2(\Omega)}$$

Airfoil problem

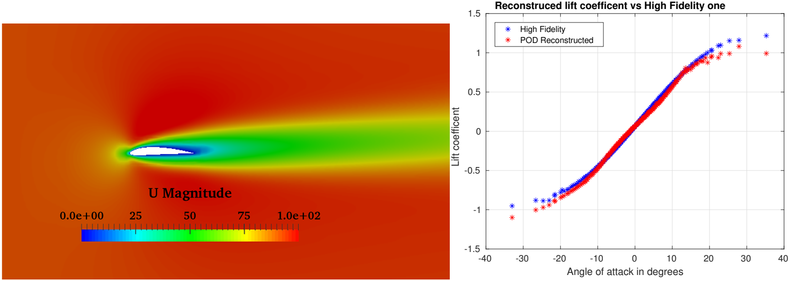


Figure: The high fidelity velocity field around the wing and the high fidelity lift coefficient versus POD reconstructed one

- A study on applying uncertainty quantification namely non-intrusive polynomial chaos expansion is being done where we aim to use POD as an evaluator output for PCE.

Under development and perspectives

- A **supremizer stabilization** technique has already been extended to a finite volume setting.
- The supremizer stabilization have demonstrated to provide **accurate results**.
- A c++ library **ITHACA-FV** based on **OpenFOAM** is under development.

Future Outlooks

- Introduce the **geometrical parametrization** in order to deal with **mesh motion** problems with the investigation of Immersed Boundary Methods.
- Study efficient methods for **affine decomposition** of the differential operators.
- Investigate the **stability** of the ROM for **long-time integration**.

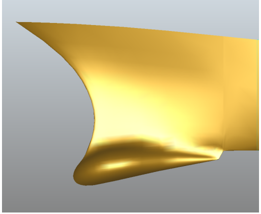
References

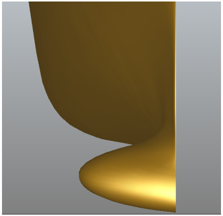
[1] G. Stabile, S. Hijazi, A. Mola, S. Lorenzi, and G. Rozza. Advances in Reduced order modelling for CFD: vortex shedding around a circular cylinder using a POD-Galerkin method. In Press, CAIM 2017

[2] G. Stabile and G. Rozza, Stabilized Reduced order POD-Galerkin techniques for finite volume approximation of the parametrized Navier–Stokes equations, submitted, 2017.

#GeometricalMorphing

Industrial FFD applications

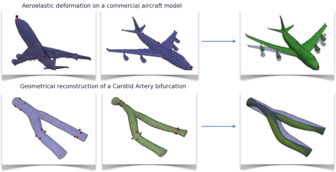


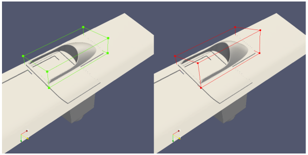


Efficient and accurate geometrical parametrization techniques

- 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 flows in the reduced basis context

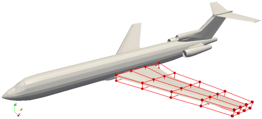
$$T(\underline{x}, \mu) : \Omega \rightarrow \Omega_0(\mu)$$

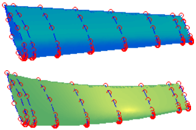




Underwater Blue Efficiency

MCY MONTECARLOYACHTS

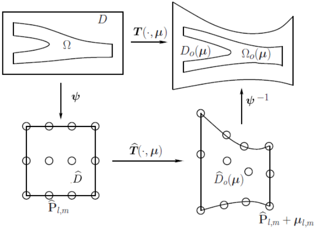




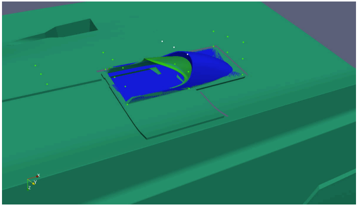
In collaboration with: F. Salmoiraghi, F. Ballarin, L. Heltai, A. Mola, M. Tezzele, N. Demo (SISSA), H. Telib, A. Scardigli (Optimad-PoliTo), D. Forti (EPFL)

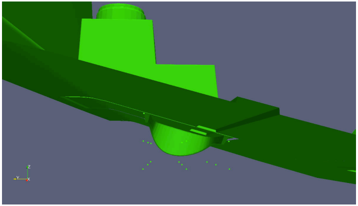
Tool for the automatic shape parametrization

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}



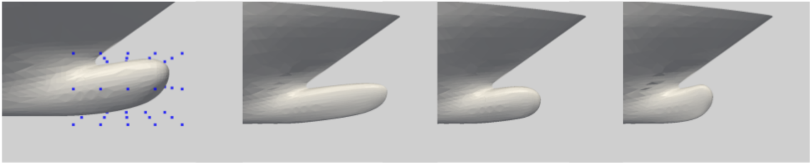
FFD: composition of the three maps $$T(\cdot,\mu) = (\psi^{-1} \circ \hat{T} \circ \psi)(\cdot,\mu)$$



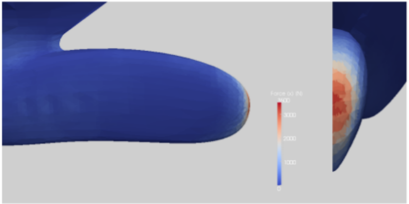


Optimisation of the shape of a bulbous bow

The hull of a ship has to break the waves easily during the navigation. For this reason, shape optimisation of the bulbous bow (the first element of a ship breaking the waves) could help in order to build efficient and high performing ships.



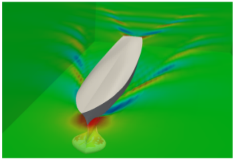
Bulbous bow

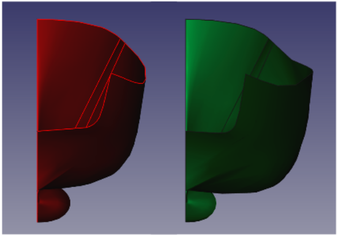


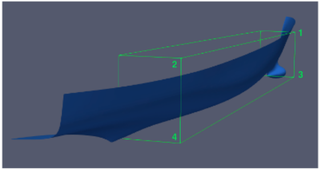
Error Analysis

Optimisation of the side of a ship

The side of the hull could be parametrized in order to verify and improve some specific characteristics (capability to transport goods and/or people) without damaging its navigation efficiency.



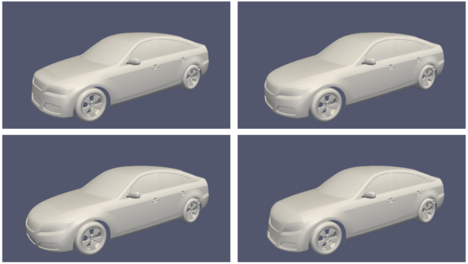




PyGeM: Python Geometrical Morphing

- 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

Conclusion

- It is time to better integrate **Data, Modelling, Analysis, Numerics, Control, Optimization and Uncertainty Quantification** in a **new parametrized, reduced and coupled paradigm**.
- **“Science and Industry advance with Mathematics”**.
- **Applied Mathematics as propeller for Innovation** and Technology Transfer.

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Thanks for your attention!

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- INDAM-GNCS 2016-2017 "Numerical methods for model order reduction of PDEs"
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Open positions on new Projects HEAD (Bormioli) and FARE-X-AROMA-CFD (compressible flows) Thanks for your attention!