Reduced-Order Models: Fundamentals and Applications



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SISSA mathLab: our current efforts, aims and perspectives

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



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Motivations

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

Leading Motivation: computational science and engineering challenges

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

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

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

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

Strategies to speed up computations:

- * High Performance Computing (HPC)
- * Model Order Reduction (MOR)



Overview of the physical parametric problems



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

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

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SISSA mathLab: our current efforts, aims and perspectives

Goals of our research group:

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



#ROM #Naval #Cardio #Environment Applications of Reduced Order Models to Naval, Biomedical and Environmental fields



Motivations: Naval Projects

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



Python package developed:





Reduction of noise generated by propellers

(in cooperation with **FLUIDS** and **CETENA**)

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

Motivations: Naval Projects

Data-driven Hull Shape Optimization System

(in cooperation with

FINCANTIERI

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



Python packages maintained:





Data-driven ROMs for blade shape optimization

(in cooperation with **FINCANTIERI**

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

Motivations: Biomedical Projects

Data-driven ROMs for patient-specific data. (in cooperation with Ospedale Luigi Sacco [])

The aim was to develop an efficient ROM framework to reduce the computational time, in order to achieve a **real time evaluation** to choose the best **surgical plan**.





Data-driven ROMs for optimal control problem. (in cooperation with University of HOUSTON)

The aim of the project is to develop a framework with the control on the **outlet boundary conditions**.



P. Siena, M. Girfoglio, F. Ballarin, G. Rozza, "Data-driven reduced order modelling for patient-specific hemodynamics of coronary artery bypass grafts with physical and geometrical parameters", 2022, arXiv preprint arXiv:2203.13682.

C. Balzotti, P. Siena, M. Girfoglio, A. Quaini, G. Rozza, "A data-driven Reduced Order Method for parametric optimal blood flow control: application to coronary bypass graft", 2022, arXiv preprint arXiv:2206.15384

Motivations: Environmental Projects

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

The interest is in geophysical flows for ocean and weather forecast. We propose a framework which combines ROM and LES, and leads to a Speed-up ≈ 100 for long time predictions.







Pollutant Control in the Gulf of Trieste

The goal is to monitor, manage and predict dangerous marine phenomena in a **fast way**. In particular we want to keep the pollutant loss under a safeguard **threshold**.

Overview

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

Intrusive Reduced Order Methods: a brief overview

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

 μ (geometry, physical properties, etc.)

- * Parametrized PDE: $\mathcal{A}(u(\mu);\mu) = r(\mu) \longrightarrow \mathcal{A}_h(\mu)u_h(\mu) = r_h(\mu) \longrightarrow \mathcal{A}^{ROM}(\mu)u^{ROM}(\mu) = r^{ROM}(\mu)$ _{reduced order}
- * Output:

$$u(\mu) pprox \mathbf{u}_h(\mu) pprox \mathbf{u}_h^{ROM}(\mu)$$
 full order reduced order

* Input-Output evaluation: (black-box) $\mu \rightarrow \mathbf{u}_{b}(\mu) \rightarrow \mathbf{u}^{ROM}(\mu)$

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

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

J. S. Hesthaven, C. Pagliantini, G. Rozza, "Reduced basis methods for time-dependent problems", Acta Numerica, 2022 G. Rozza, G. Stabile, F. Ballarin, "Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics", SIAM Press, 2022 Intrusive Reduced Order Methods: a brief overview

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

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

ROMs: libraries developed at SISSA mathLab (software)

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



¹mathlab.sissa.it/cse-software

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> **#POD #RB #continuation** #timeline #wind-engineering #pioneers Acknowledgements: Luca Bruno

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Model Order Reduction: Historical Perspectives

Two historical approaches:

- Proper Orthogonal Decomposition (POD) to simulate time dependent flows and as efficient way to model turbulent flows ¹ ²
- Reduced Basis Methods as continuation methods in non-linear structural mechanics 3 4 5

At the state of the art these two approaches are also merged.

• Other methods: Principal Generalized Decomposition (PGD), Hierarchical Model Reduction (HMR), 67



¹Ravindran. S. S. (2000). A reduced-order approach for optimal control of fluids using proper orthogonal decomposition. International journal for numerical methods in fluids. 34(5), 425-448.

²Sirovich, L. (1987). Turbulence and the dynamics of coherent structures. I. Coherent structures. Quarterly of applied mathematics. 45(3), 561-571.

³Noor, A. K., & Peters, J. M. (1980). Reduced basis technique for nonlinear analysis of structures. AIAA Journal, 18(4). 455-462

⁴Noor, A. K., (1982). On making large nonlinear problems small, Computer Methods in Applied Mechanics and Engineering 34.955 - 985.

⁵Fox. R.L. and Miura. H. (1971). An approximate analysis technique for design calculations, AIAA Journal 9, 174–179.

⁶Benner, P., Schilders, W., Grivet-Talocia, S., Quarteroni, A., Rozza, G., & Miguel Silveira, L. (2020-2021). Model Order Reduction: Volumes 1.2.3. De Gruvter.

⁷Stein. E., De Borst, R., Hughes, T. J. (2004). Encyclopedia of computational mechanics, Model Order Reduction, Wiley. ⁸Chinesta, Huerta, Rozza, Willcox, Encyclopedia Comp. Mechanics, 2015

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Historical contributions and challenges

- After few attempts in the 80's, only after 2000's, when computational resources were available, there was a new era for Reduced Order Methods^a.
- * Several research groups developed in Europe and North America in aeronautics/astronautics/mechanical engineering department/applied mathematics focused on ROMs.



- Nowadays several initiatives at the European level contributed in the consolidation of the community (COST EU-MORNET).
- * In ECCOMAS/SIAM congresses several sessions are now dedicated to ROMs and applications.



^aThere was lack of computational power for offline steps because Numerical Analysis was still far to provide efficient tools.

ROM developments



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

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Building the Reduced Space: POD vs RB

Full Order Model: $A_h(\mu)u_h(\mu) = r_h(\mu)$ with **Parameters** in a training set: $\mu_i \in [\mu_1, \dots, \mu_{N_t}]$

Proper Orthogonal Decomposition:

- Solve FOM for all training set $\boldsymbol{u}_h^i = \boldsymbol{u}_h(\boldsymbol{\mu}_i)$
- Eigenvalue problem:

$$oldsymbol{\mathcal{C}}_{ij} = (oldsymbol{u}_h^i)^Toldsymbol{\mathcal{M}}oldsymbol{u}_h^j \quad o \quad oldsymbol{\mathcal{C}}oldsymbol{\mathcal{V}} = oldsymbol{\mathcal{V}}oldsymbol{\lambda}$$

• Keep the most energetic N_r POD modes:

$$\boldsymbol{\xi}_{i}(\boldsymbol{x}) = \frac{1}{N_{t}} \sum_{j=1}^{N_{t}} \boldsymbol{V}_{ji} \boldsymbol{u}_{h}^{j}(\boldsymbol{x}) \text{ for } i = 1, \dots, N$$
$$\Xi = [\boldsymbol{\xi}_{1}, \cdots, \boldsymbol{\xi}_{N_{r}}] \in \mathbb{R}^{N_{h} \times N_{r}}$$

Optimal in $|| \cdot ||_2$ sense

$$\mathbf{u}_h \in \mathbb{V}_h$$
 and $dim(\mathbb{V}_h) = N_h$

Reduced basis:

• We provide an error estimator $\eta(\mu, \Xi)$

•
$$\Xi := \{ \boldsymbol{u}_h(\boldsymbol{\mu}_0) \}$$

- Iteratively
 - Find largest error

$$\eta(oldsymbol{\mu}^*, \Xi) = \max_i \eta(oldsymbol{\mu}^i, \Xi)$$

 $\Xi =: \{\Xi, u_h(\mu^*)\}$

Expand

Optimal in $|| \cdot ||_{\infty}$ sense

• Reduced solution: $u^{ROM}(\mu) = \sum_{i=0}^{N_r} u_i^R(\mu)\xi_i(\mathbf{x}), \quad u^{ROM}(\mu) = \Xi u^R(\mu) \text{ for } u^R \in \mathbb{R}^{N_r}$

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

Reducing the model

Full Order Model: $A_h(\mu)u_h(\mu) = r_h(\mu)$ with $u_h \in \mathbb{V}_h$ and $dim(\mathbb{V}_h) = N_h$ **Reduced space:** Ξ

Galerkin projection:

• Reduced solution:

$$oldsymbol{u}^{ROM}(oldsymbol{\mu}) = \sum_{i=0}^{N_r} u^R_i(oldsymbol{\mu}) oldsymbol{\xi}_i(oldsymbol{x}) = \Xi oldsymbol{u}^R$$

• Project on the left:

$$\underbrace{\Xi^{\mathsf{T}} \mathbf{A}_{h}(\mu) \Xi}_{\mathbf{A}^{ROM}(\mu) \in \mathbb{R}^{N_{r} \times N_{r}}} \mathbf{u}^{R}(\mu) = \underbrace{\Xi^{\mathsf{T}} r_{h}(\mu)}_{r^{ROM}(\mu)}$$

• ROM $\boldsymbol{A}^{ROM}(\mu)\boldsymbol{u}^{R}(\mu) = r^{ROM}(\mu)$

Regression technique:

• Find some values for the map

 $oldsymbol{\mu} o oldsymbol{u}^{\scriptscriptstyle R}(oldsymbol{\mu})$

for example on training set $oldsymbol{u}^R(oldsymbol{\mu}^i)$

- Approximate the map $u^R(\mu)$ with $\hat{u}^R(\mu)$
 - Neural Networks
 - Interpolation functions
 - Least square approximations
 ...
- ROM is the evaluation of $\hat{u}^{R}(\mu)$

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

Challenges and Frontiers

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

Strategic Fields of development for ROMs

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









ROM challenges in CFD

Classical Discretization techniques:



increasing Reynolds number





Key problems:

- * Stabilization issues and fulfillment of *inf-sup* condition
 - stabilization approaches (SUPG, variational multi-scale approach)
 - SUP-ROM: addition of supremizer modes to enrich the velocity space
 - PPE-ROM: replacement of the continuity equation with the pressure Poisson equation

* Turbulence treatment

 Reliability of classical and reduced discretization methods in real world applications

ROM challenges in CFD

Other options:





Key problems:

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

Stabilization techniques for FEM-based ROM

FEM (Finite Element Method)

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



¹What is the *inf-sup* condition?

Consider the saddle-point problem:

Find u in V, p in Q such that, $\forall v \text{ in } V \text{ and } \forall q \text{ in } Q$:

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

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

$$\begin{split} & \inf_{q \in \mathcal{Q}, q \neq 0} \sup_{v \in V, v \neq 0} \frac{b(v,q)}{\|v\|_{V} \|q\|_{Q}} \geq \beta, \\ & \beta \geq 0. \end{split}$$

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

Stabilization techniques for FV-based ROM

- lack of accuracy in pressure recovery with standard POD-Galerkin approaches
- stabilization techniques:
 - **SUP-ROM**: introduction of supremizer modes $\mathbf{s}_i = \mathbf{s}(\chi_i)$ (where χ_i are the pressure modes) such that:

$$\begin{cases} \Delta \mathbf{s}_i = -\nabla \chi_i \text{ in } \Omega \\ \mathbf{s}_i = \mathbf{0} \text{ on } \partial \Omega \end{cases}$$

• **PPE-ROM**: replacement of the continuity equation with the pressure Poisson equation

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

• Variational Multi-Scale ROM approach: introduction of data-driven *correction* terms in the reduced system.



FVM (Finite Volume Method)

Stabilization techniques: the Variational Multi-Scale (VMS) ROM approach

When building a Reduced Order Model, different modal regimes can be chosen:

- under-resolved regime: fewer ROM modes than the number required to accurately approximate the dynamics of the flow:
- marginally-resolved regime: the number of ROM basis functions is enough to represent the main features of the system, but the standard G-ROM yields inaccurate approximations:
- fully-resolved regime: the number of modes is enough to represent the underlying dynamics of the system.

How to improve the accuracy in the marginally-resolved regime?

Include the contribution of the neglected modes in the ROM by adding extra correction/closure terms

Standard ROM DD-VMS-ROM

 $egin{array}{lll} \dot{\mathbf{a}} = f(\mathbf{a},\mathbf{b})\,, & & & & & \\ egin{array}{lll} \dot{\mathbf{a}} = f(\mathbf{a},\mathbf{b}) + oldsymbol{ au}_u\,, & & & \\ eta(\mathbf{a},\mathbf{b}) = oldsymbol{0}\,. & & & & & \\ eta(\mathbf{a},\mathbf{b}) = oldsymbol{ au}_{
ho}\,, & & & & \\ \end{array}$

where **a** and **b** are the reduced coefficient vectors for velocity and pressure.



Ivagnes, A., Stabile, G., Mola, A., Iliescu, T., & Rozza, G. (2022). Pressure Data-Driven Variational Multiscale Reduced Order Models, arXiv preprint arXiv:2205.15118.

Artificial Intelligence: CSE applications with neural networks

Artificial Intelligence can be applied in several fields of Computational Fluid Dynamics and Model Order Reduction.

Feedforward Neural Networks

Used as regression technique for:

- approximation in reduced order models (POD-NN)
- inclusion of turbulence modelling in non-intrusive reduced order models





Autoencoders

- dimensionality reduction
- features extraction

Meneghetti, L., Demo, N., & Rozza, G. (2021). A Dimensionality Reduction Approach for Convolutional Neural Networks. arXiv preprint arXiv:2110.09163.

Romor, F., Stabile, G., & Rozza, G. (2022). Non-linear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method. arXiv preprint arXiv:2203.00360.

Artificial Intelligence: physics informed CSE applications

Convolutional Neural Networks

- object detection
- image recognition





PINA: a Python package for the approximated resolution of PDEs and ODEs with physics-informed neural networks. https://cithub.com/amthlab/PINA

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Analytical solution (left), PINN solution (right) to a Poisson problem.

Physics-Informed Neural Networks

- inclusion of the physical laws and governing equations in the loss function
- strategy to approximately solve PDEs

Meneghetti, L., Demo, N., Rozza, G., & Sonego, M. Convolutional Neural Networks for object detection in professional appliances.

Demo, N., Strazzullo, M., & Rozza, G. (2021). An extended physics informed neural network for preliminary analysis of parametric optimal control problems. arXiv preprint arXiv:2110.13530.

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ROM for turbulent flows (Zancanaro et al.)

Why not a Direct Numerical Simulation?

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

Involved conservation laws: Reynolds averaged Navier-Stokes equations

$$\begin{cases} \nabla \cdot (\overline{\boldsymbol{u}} \otimes \overline{\boldsymbol{u}}) - (\nu + \nu_t) \nabla^2 \overline{\boldsymbol{u}} + \nabla \overline{p} + \frac{2}{3} \nabla k = 0\\ \nabla \cdot \overline{\boldsymbol{u}} = 0 \end{cases}$$
(1)

where $\nu = \mu/\rho$ is the kinematic viscosity, ν_t stands for the eddy viscosity while k represents the turbulent kinetic energy, being $\overline{u} \in \mathbb{V}_h$ and $\overline{p} \in \mathbb{Q}_h$.



Turbulent flows - Turbulence treatment

The reconstruction of the eddy viscosity field can be done with a fully-connected neural network².



Reduced eddy viscosity field: $\nu_{tr} = \sum_{i=1}^{N_{\nu_t}} m_i(\mathbf{x})\zeta_i(\boldsymbol{\mu}),$ where: * $\mathbf{m} = (m_i)_{i=1}^{N_{\nu_t}}$ is the eddy viscosity coefficient vector; * $(\zeta_i)_{i=1}^{N_{\nu_t}}$ are the eddy viscosity modes. Mapping from known modes:

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

Neural network mapping:

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

Loss function of the neural network

$$\mathcal{L} = \sum_{i=1}^{N_{
u_t}} ||m{m}_i - m{ ilde{m}}_i||_{L^2}$$

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

DATA

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Conclusions

- * It is time to better integrate Data, Modelling, Analysis, Numerics, Control, Optimization and Uncertainty Quantification in a new parametrized, reduced and coupled paradigm;
- * we need to draw the attention to the fact that "Science and Engineering could advance with Mathematics (CSE)";
- * Applied Mathematics as propeller for methodological innovation and technology transfer by a new generation of talented computational scientists.



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- * COST, European Union Cooperation in Science and Technology, TD 1307 EU-MORNET Action
 (http://www.eu-mor.net)
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- * H2020 MSCA EID ROMSOC,2019-2022;
- * SMACT;
- * FSE FVG;



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