

ADVANCES IN REDUCED ORDER METHODS FOR PARAMETRIC INDUSTRIAL PROBLEMS IN COMPUTATIONAL FLUID DYNAMICS

G. ROZZA¹, M.H. MALIK¹, N. DEMO¹, M. TEZZELE¹, M. GIRFOGLIO¹,
G. STABILE¹ AND A. MOLA¹

¹ SISSA International School for Advanced Studies, Mathematics Area, mathLab,
Via Bonomea 265, 34136 Trieste, Italy
{gianluigi.rozza, mmalik, ndemo, mtezzele, mgirfogl, gstable, amola}@sissa.it,
<http://mathlab.sissa.it>

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Abstract. Reduced order modeling has gained considerable attention in recent decades owing to the advantages offered in reduced computational times and multiple solutions for parametric problems. The focus of this manuscript is the application of model order reduction techniques in various engineering and scientific applications including but not limited to mechanical, naval and aeronautical engineering. The focus here is kept limited to computational fluid mechanics and related applications. The advances in the reduced order modeling with proper orthogonal decomposition and reduced basis method are presented as well as a brief discussion of dynamic mode decomposition and also some present advances in the parameter space reduction. Here, an overview of the challenges faced and possible solutions are presented with examples from various problems.

1 INTRODUCTION AND MOTIVATION

Advances in computational capabilities and the computational power of modern computer systems lead to more accurate and complex mathematical and numerical models. These ever increasing complexity is coordinated with the progress in the modeling, numerical analysis and faster algorithms in computational science. Despite all the advancements, there are still several problems in science and engineering which are relatively difficult to be computed [1]. The various challenges faced during can be summarized as:

- The first challenge is handling of the higher dimensional space. Models with definition in high dimensional spaces encounter what is called “curse of dimensionality”, examples of such problems are many parametric problems.
- On-line control of complex systems, which requires fast real time simulations usually on hand held devices such as tablets.

- Problems involving inverse identification, process and shape optimization.

This list provides very basic examples and in practical there are many more challenges that remain out of the reach of traditional computational strategies. There are two possible solutions to these challenges; the first is to reduce the complexity of the mathematical model by introducing assumptions in the physics of the problem to simplify the mathematical model, but this approach is not always practical and can also be the cause of introduction of errors. The second approach is the utilization of High Performance Computing (HPC) [2], which has its own drawback as HPC is expensive to install and immobile. A more suitable approach is the development of reduced order models, which relies on the division of the problem such that a complex and higher order problem is solved with greater accuracy using expensive computational facilities normally during off-line phase and then using fast on-line phase to compute specific solutions on much less computational expense.

Reduced order modeling relies on the mathematical approach rather than introducing assumptions to simplify the problem [2], to obtain much smaller model than the high fidelity model without compromising the accuracy of the solution. There are a number of techniques available for the purpose of model order reduction; categorized into two types; *a posteriori* and *a priori*. A posteriori model order reduction method includes proper orthogonal decomposition (POD) [3, 4], trajectory piecewise linear method (TPWL) [5, 6], reduced basis (RB) method [7, 8, 9] including also tools like empirical interpolation method (EIM) [10] to name a few. A priori model order reduction methods include methods such as proper generalized decomposition (PGD) [11, 12] and a priori reduction method (APR) [13, 14].

In this manuscript, the authors present an overview of various applications of reduced order modeling techniques with the focus on computational fluid dynamics (CFD). The paper is organized as Section 2 provides the recent advances in the reduced order modeling, from Section 3 to Section 9 we present, application of reduced order modeling (ROM) in several scientific and industrial applications.

2 ADVANCES IN REDUCED ORDER MODELING

With the recent advances in the computational science, the focus of research is more towards the development of numerical methods and strategies for the parametric problems involving partial differential equations (PDEs). The introduction of parameters as discussed in Section 1 increases the dimension of the problem space, the parameters can arise from material, geometrical and non-dimensional coefficients. The research in the fields of numerical analysis specifically in computational mechanics with applications such as simulation, optimization and real time control deals with such parametrized PDEs. Such cases require multiple numerical solutions of PDEs with different parameter values which require high computational efficiency. These problems, therefore, provide the need for development of reduced order modeling techniques such as RB, POD and PGD.

Reduced basis methods [15] have been developed into a strong model order reduction method in previous years providing reduction of computational times for the solution

of parametrized PDEs. Similar to most of model reduction techniques, reduced basis methods divide the solution in an off-line stage and an on-line stage. In the off-line stage, a solution is sought of the high fidelity model; of the order, say N ; with the help of suitable discretization technique finite element method (FEM), finite volume method (FVM) and finite difference (FD) etc., depending upon the nature of the problem. During this stage, a number of solutions are stored for different parameter values which are chosen in an optimal way and are subsequently used to generate a reduced basis of much smaller order $M \ll N$. Once the off-line phase is completed, reduced basis functions can be utilized for the generation of new solutions for new parameter values combining the previously computed basis functions by means of a Galerkin projection [15, 16] in a fast and efficient manner. This problem in reduced dimensional space is very small and therefore useful in the deployment of real time scenarios. The solution thus obtained is reliable and accurate ensured by residual-based a posteriori error estimates.

Recent research activities in the field of reduced order modeling prove the effectiveness of this approach and has resulted in significant development of model order reduction methods for several different problems of practical interest [17]. For engineering applications, in addition to be able to perform efficient numerical simulations for complex geometries of various different materials, reduced order methods need to be capable of parameterizing the geometric shape of the structure itself. Similar, requirements are also found in medical applications for example the CFD analysis of blood flow through vessels [18, 19]. Current focus of the research is towards developing the theory and the methodology of reduced order methods for computational fluid dynamics for different physical and temporal scales and also for complex nonlinear problems such as bifurcations and instabilities. On a vastly different scale from the blood flows [20, 19] and biology of singular cell and micro-organisms [21], is the application in the naval and nautical engineering. As well as there are applications in well defined CFD problems of aerospace, mechanical and automotive engineering and porous media and geophysics.

These developed reduced order methods can be used in combination with techniques in data assimilation and uncertainty quantification for the solution of complex inverse problems found in the multidisciplinary fields described here.

3 CFD WITH FINITE VOLUME METHOD

The finite volume method is particularly widespread in several engineering fields (aeronautics engineering, naval engineering, automotive engineering, civil engineering, ...) and historically is widely used in industrial applications characterized by higher values of the Reynolds number, refer Figure 1 for typical examples. The finite volume method rather than operating on the strong form of the equations works on the integral version of the equations. Divergence terms are then converted into to surface integrals exploiting the divergence theorem and the conservation law is enforced in each finite volume. For more details concerning the derivation of the discretized equations and the mathematical foundations of the method the reader may see [22, 23]. However, in the field of reduced order methods, this discretization technique is usually less employed respect to the finite element method. To this purpose, one of the first contribution dealing with finite volumes

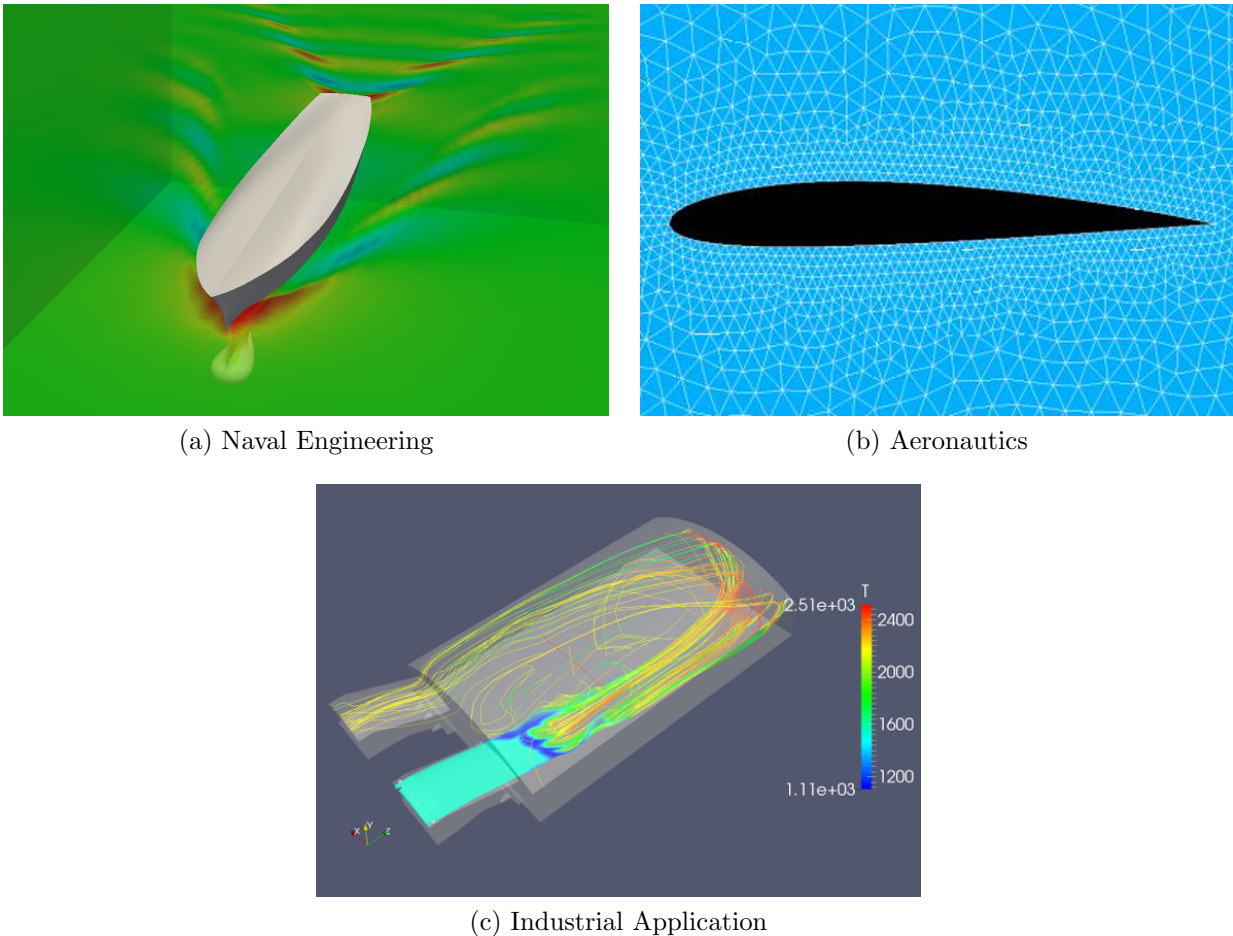


Figure 1: Possible applications where the finite volume discretization is particularly widespread

and the reduced basis method, in the context of a linear evolution equations, can be found in [24]. A recent contribution considering non-linear evolution equations modeling fluid dynamics problems can be found in [25], in [26] pressure stabilization techniques normally employed in a FEM-based POD-Galerkin methods are extended to a finite volume framework while [27] proposes a new ROM where conservation laws are enforced also at the reduced order level. The implementation of ROMs for finite volume schemes will allow to more effectively propose the reduced order methodology outside the academic environment for complex and real-world problems that industrial partners face on a daily basis. Recently the open-source library ITHACA-FV [28] has been released which is based on OpenFOAM [29], the most widely used general purpose open-source CFD software package.

3.1 Some ROM challenges in CFD for finite volume scheme

In the last years some progresses have been achieved but there are still several issues that need to be tackled. Among them, the most challenging ones are ROMs for turbulent

flows and ROMs that include geometrical parametrization. Regardless from the starting full order discretization technique, the majority of projection based ROMs are limited to laminar flows and relatively few reports for turbulent flows have appeared in the literature and here we report some of the most relevant [30, 31, 32, 33, 34]. Among these works only few are based on finite volumes, on the contrary, at full order level, a large variety of closure models for turbulent flows can be found. For this reason it is crucial to export what has been done for full order finite volume schemes to a reduced setting. Concerning geometrical parametrization, in finite elements, a common strategy is the usage of equation written into a reference domain in order to have all the results in a common domain. This approach is however not easy to be transferred to a finite volume setting and in many cases even not possible. In fact, dealing with non-linear and non-explicit schemes, or with complex geometrical deformations, this operation becomes not possible. Possible ways to overcome this limitation could rely on the usage of immersed methods [35]. In this way is possible to write all the equations on the same physical domain and to treat the immersed structure as an external forcing term.

4 DYNAMIC MODE DECOMPOSITION

Dynamic mode decomposition (DMD) is an emerging tool for complex systems analysis. Initially introduced in the fluid dynamics community [36], this technique has been adopted also in many other fields due to the capability to represent a complex — also nonlinear — system as linear combination of few main structures that evolve linearly in time. Since DMD approximates the Koopman operator [37] using just the data extracted from the underlying system, this method does not require any information about the governing equations. Due to its diffusion, in the last years several variants of the standard algorithm have been developed, like multiresolution DMD [38], forward-backward DMD [39], higher order DMD [40] and compressed DMD [41]. All these variants have been implemented in an open source Python package called PyDMD [42]. An example of the PyDMD application on a fluid dynamics simulation is shown in Fig 2.

Basically, we want to approximate the Koopman operator \mathbf{A} such that it can simulate the system time evolution, hence the relation between two sequential instants is $\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k$, where \mathbf{x}_i denotes the state at i -th instant. To achieve this, we collect a series of data vectors containing the system states, from now on *snapshots*, and arrange them into two matrices such that $\mathbf{S} = [\mathbf{x}_1 \ \dots \ \mathbf{x}_{m-1}]$ and $\dot{\mathbf{S}} = [\mathbf{x}_2 \ \dots \ \mathbf{x}_m]$. The linear operator is built to minimize the error $\|\dot{\mathbf{S}} - \mathbf{A}\mathbf{S}\|$, so $\mathbf{A} = \dot{\mathbf{S}}\mathbf{S}^\dagger$, where † refers to the Moore-Penrose pseudo-inverse. To avoid handling this large matrix, the reduced operator is computed. The matrix \mathbf{A} is projected on the space spanned by the left-singular vectors of matrix \mathbf{S} , found by the truncated singular value decomposition (SVD), that is $\mathbf{S} \approx \mathbf{U}_r \Sigma_r \mathbf{V}_r^*$. Once we obtained the reduced operator $\tilde{\mathbf{A}}$, we can reconstruct the eigenvectors and eigenvalues of the matrix \mathbf{A} thanks to the eigen-decomposition of $\tilde{\mathbf{A}}$, which is $\tilde{\mathbf{A}}\mathbf{\Lambda} = \mathbf{\Lambda}\mathbf{W}$. In particular the elements in $\mathbf{\Lambda}$ correspond to the nonzero eigenvalues of \mathbf{A} , while the real eigenvectors, the so called exact modes [43], can be computed as $\Phi = \dot{\mathbf{S}}\mathbf{V}_r \Sigma_r^{-1} \mathbf{W}$.

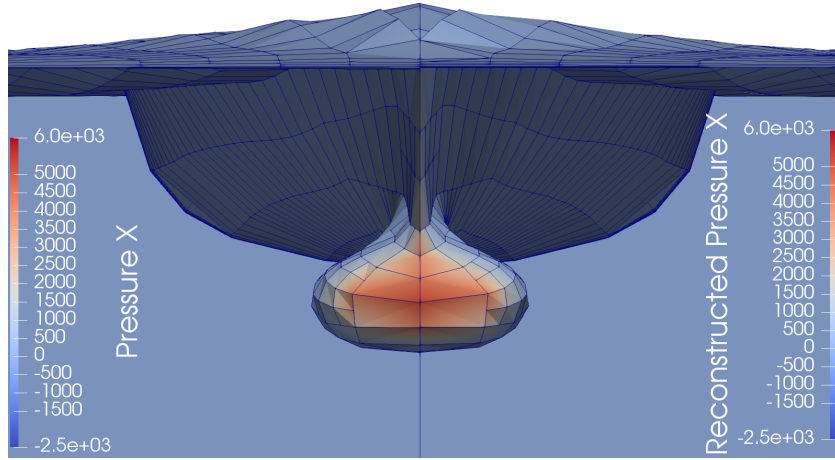


Figure 2: Application of DMD on a naval simulation: on the left the high-fidelity solution, on the right the points displacement and the pressure field reconstructed.

5 PROPER ORTHOGONAL DECOMPOSITION WITH INTERPOLATION

Within the model reduction techniques, the proper orthogonal decomposition interpolation (PODI) method is exploited both in the academia and industrial context for the real time approximation of the solution of parametric partial differential equations [44, 45, 46, 47, 48]. Since it relies only on the high-fidelity solutions, its biggest advantage is to be completely independent from the full-order solver and to not require any assumptions on the underlying system.

Initially, in the PODI approach, the parametric space \mathbb{D}^N is sampled and the high-fidelity solutions are computed by solving the full-order model built using these parametric points. At this stage, the numerical method and the discretization can be chose to reach the desired accuracy. Once these solutions are collected — the most expensive phase — we can represent them as a linear combination of few main structures, the so called POD *modes*. The modes correspond to the left-singular vectors individuated by applying the singular value decomposition (SVD) to the solutions matrix. We define the *modal coefficients* as the projection of the high-fidelity solutions onto the space spanned by the modes: thanks to the correlation between the parametric points and the modal coefficients, we can interpolate the solution for any parameter point that belongs to \mathbb{D}^N . Even though the accuracy of the approximated solution depends from the interpolation method used, the capability to generate the reduced model using only the system output make this equation-free algorithm specially suited for the industrial applications. About this, the PODI method has been proposed and implemented by the mathLab group in an open-source package on Github, called EZyRB [49].

6 EFFICIENT GEOMETRICAL PARAMETERIZATION TECHNIQUES IN THE CONTEXT OF ROM

Nowadays shape optimization has gained a lot of interest. In this framework an efficient and accurate geometrical parametrization is a critical part for each optimal shape

design simulation campaign. This is true especially in the context of reduced order modeling, where it is possible to discern the shape morphing methods in two main groups: *general purpose* or *problem specific*. While the later aims at reducing the parameter space using specific characteristics of the problem at hand, like, for instance, the centerlines-based approach proposed in [19], the first approach applies to a wide range of problems. Among possible *general purpose* methods we mention *Free-Form Deformation* (FFD) [50, 51, 52, 47], *Radial Basis Functions* (RBF) interpolation [53, 54, 55] or *Inverse Distance Weighting* (IDW) interpolation [56, 57, 58]. These methods identify the parameters as the displacements of some control points that define the morphing of the domain. All the aforementioned techniques are implemented in an open source Python package called PyGeM [59]. Earlier approaches to parameter space reduction relies on modal analysis [58], screening procedures based on Morris' randomized one-at-a-time design [60, 61], or semi-automatic reduction of the number of control points [62]. The reduction of the parameter space is achieved by retaining an optimal subset of the possible control points. This can result in a set of admissible deformations too shrunk. This can be overcome in part with the use of active subspaces as explained in the following section. Another issue is the optimal position of such control points. We underline that the FFD is very versatile since it can be easily integrated into existing software pipelines for CFD simulations, simply constructing a lattice of points around the part of the domain to be morphed. In particular PyGeM software can deal with a variety of file formats for both academic and industrial purposes.

7 NEW ADVANCES IN PARAMETER SPACE REDUCTION WITH ACTIVE SUBSPACES

The improved capabilities in terms of computational power of the last decade has led to more and more sophisticated CFD simulations. Increasing the number of parameters allows finer sensitivity analysis, and expand the design space to explore for shape optimization problems. To fight the curse of dimensionality a possible approach is to reduce the dimension of the parameter space. In the last years the active subspaces technique, introduced in [63], has been employed with success in many different engineering problems such as optimal shape design [64], hydrologic models [65], naval engineering [66, 67], and uncertainty quantification [68]. Active subspaces are a property of a parametric multivariate scalar function, representing the quantity of interest, and a probability density function used to sample the parameter space. An active subspace is the span of the eigenvectors of the uncentered covariance matrix of the gradients of the target function with respect to the parameters. In practice the new reduced parameters are a linear combination of the original ones, that accounts for how much the quantity of interest varies along each parameter direction. It can also be thought as a rotation of the parameter space in order to unveil a lower dimensional behavior of the function of interest. The insights given from the active subspace of a function are multiple: it is possible to identify the more important parameters, and the ones we can discard without affecting too much the approximation. This allows an efficient choice of the geometrical parameters in optimal shape design problems where the parametrization of the design is crucial together with

the exact choice of the parameters to describe it.

New advances have been made for what concerns time dependent functions [69], the combination with POD-Galerkin model reduction for cardiovascular problems [70], the extension to vector-valued functions [71], and the combination of different active subspaces of different functions [72]. Since, to find an active subspace, we need couples of input/output data, the technique can be easily integrated within existing pipelines consisting, for example, on geometrical parametrization and equation-free reduction techniques as in [67]. Other approaches are possible to perform design-space nonlinear dimensionality reduction, for a comparative review we suggest [73], while for an application to naval engineering and shape optimization we cite [74].

8 NAVAL AND NAUTICAL ENGINEERING APPLICATIONS

In the last decade, naval and nautical engineering fields have witnessed a progressive introduction of high fidelity hydrodynamic simulations into the design process of ship hulls, propellers and other components. The increased computational capabilities and the wealth of reliable simulation models and softwares, nowadays allows for the evaluation of the fluid dynamic performance of virtual models designed by the engineer. Such new virtual prototyping scenarios propel the demand of new instruments which would make the design pipeline more efficient. First, since many high fidelity CFD simulations are typically carried out during a design campaign, engineers now need reliable instruments to automatically produce a suitable set of geometries which can be readily converted into quality computational grids, and can at the same time explore in the most extensive way the space of possible designs, in search for the optimal one. The production of new shapes to be tested in fact, is in the most common practice carried out by skilled designers who manually operate CAD tools to obtain shapes that can improve hydrodynamic performance and still fulfill the structural and bulk/volumetric constraints to which the components are subjected. In addition to such time consuming task, the geometries generated must be imported into mesh generation tools to obtain suitable computational grids for CFD simulations.

Part of the current work at mathLab is focused on the development of algorithms for the shape parametrization different components of the ship considered in the design process. In such framework, both FFD implemented in the PyGeM software and specifically developed shape deformation strategies are applied to ship and planing yacht CAD geometries, resulting in a series of parametrized IGES geometries. For each morphed shape, we compute a series of geometrical and hydrostatic parameters which are of typical interest of the naval and nautical engineers. This allows for a first selection of the shapes that will be tested, which avoid running detailed CFD simulation on configurations that are *a priori* known to be unsatisfactory. As some mesh generators in the CFD community operate starting from STL triangulations —as do 3D printers— a surface mesh generator has been implemented to obtain water tight triangulations on non water tight hull geometries. In addition, a further tool which employs PyGeM FFD and RBF tools to directly deform the volumetric meshes generated on the original hull shape is being developed. This will further reduce the amount of human interaction required to carry

out a simulation campaign. As for the marine propeller shape parametrization, a specific tool has been developed to build bottom-up propeller virtual model in which the blades are parametrized on the camber and thickness of the airfoils used, as well as the rake, skew, pitch and chord distribution as a function of the radial coordinate. The result of the procedure is represented by the IGES geometry of the propeller, and the corresponding STL water-tight triangulation.

Along with the pre-processing tools described, the work is focusing both on the development of reduced order models aimed at reducing the computational cost of the hydrodynamics simulation campaign, and on a smart post processing of the CFD simulations output based on active subspaces. As for the first task, we are currently applying PODI tools included in the ITHACA-FV to RANS ship hydrodynamic simulations carried out with OpenFOAM. When a restricted amount of parameters are considered, such model reduction strategy is in fact able to provide reliable predictions of the entire flow field. For cases in which more parameters have to be considered, more conventional POD approaches are being considered. Once all the simulations have been carried out, the relationship between input and output parameters is studied to identify the presence of active subspaces. This information obtained from such analysis is particularly relevant to design engineers. It in fact is able to trigger possible redundancies in the parameter space and, in some cases, it can also provide some physical insight on the possible correlation among some parameters involved in the design process. As mentioned, a first application of the entire pipeline composed by shape parametrization, high fidelity computations and post processing analysis with active subspaces has been presented in [74].

9 INDUSTRIAL ENGINEERING APPLICATIONS

New simulation frameworks are required for the analysis of industrial engineering problems that often involve multi-physics systems governed by sets of coupled PDEs. A typical example belonging to this category is the fluid structure interaction (FSI) that deals with the investigation of the interaction phenomena between deformable or movable structures with a surrounding (Figure 3) or internal (Figure 4) fluid flow. The treatment of such problems requires the introduction of proper coupling conditions as well as the development of adequate numerical algorithms. The scientific literature includes a lot of works focused on the interaction between an incompressible fluid flow and an hyperelastic solid but it should be noted that industrial problems often are characterized by a very complex multi-physics scenario which involves combined effects of turbulent flows, thermo-chemical reactions, multiphase and interfacial flows. Further elements of complexity that can be present in industrial applications are for instance multiple regions separated by multiple interfaces [75].

Regarding the full order model, the numerical procedures to solve FSI problems may be classified into two categories: monolithic and partitioned. In the monolithic approach, flow and structure equations are solved simultaneously with a single solver and the interfacial conditions are implicit in the solution procedure [78], whilst in the partitioned approach flow and structure equations are solved in sequence with two distinct solvers and the interfacial conditions are used explicitly to communicate information between the fluid

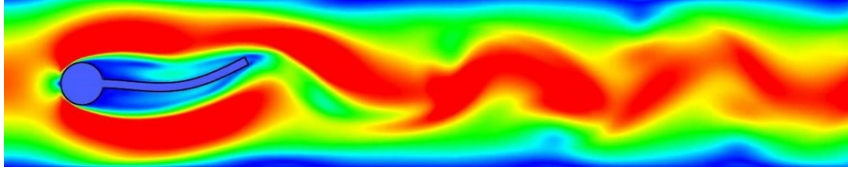


Figure 3: Simulation of the Hron and Turek FSI benchmark [76].

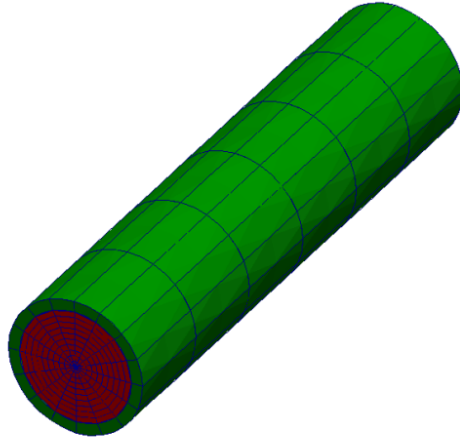


Figure 4: Flexible tube benchmark problem with the employed fluid (red) and solid (green) computational grids [77].

and structure solutions [79]. Of course reduced order models should be considered related to both approaches.

In the industrial context, the partitioned approach is the most broadly used; it preserves software modularity because existing solvers are coupled. Then, different and more efficient techniques developed specifically for solving flow and structure equations can be readily employed. Of course, the development of stable and accurate coupling algorithms is required in partitioned approaches. In particular, depending on the physics nature of the interaction, one-way or two-way coupling procedures are demanded; in the former case transfer quantities are sent from one domain to the other but not in the opposite direction, in the latter one the solver data is always transferred both ways at the fluid-structure interaction. Moreover, due to the strength of the coupling that can occur in some problems as well as the well known problem of the artificial added mass [80], that introduces further instabilities, a partitioned approach often requires to iterate the solution process of the systems of equations several times every time step by determining a significant increase of the computational cost. Quasi-Newton methods [81] are an example of efficient iterative methods that have been employed in order to ensure a low number of iterations. The numerical treatment of the interaction of a fluid and slender structures is a very challenging problem [82]. Proper Orthogonal Decomposition (POD) reduced order models have been built on a strong coupling algorithm for partitioned FSI approaches

in order to improve the convergence rate of the iterative method when a lot of previous iterations are reused [77]. In [83], authors show that Singular Value Decomposition (SVD) is also a very useful and robust algorithm to treat the ill conditioning of the linear system involved by an iterative method. A recent approach is presented in the study by Ballarin et al [84].

Monolithic approaches can potentially achieve better stability and convergence properties but they require the development and handling of a specialized code. Of course they are more robust for strongly coupled problems but it has been shown that the monolithic approach allows to obtain a good performance even for problems characterized by a weak coupling [85]. Some preliminary features of monolithic reduced order models for FSI problems have been investigated in [86].

10 CONCLUSIONS

With this manuscript, we have presented some examples of recent advances in research activities of mathLab, SISSA group in various domains focusing on the application of model order reduction techniques. The recent developments in the area of model order reduction methods are now on a level where there is better capability to face much more complex problems. It is now possible to include data driven modeling within the analysis, control and optimization. As discussed in this manuscript, now model reduction techniques are applied to several industrial engineering applications, as demonstrated by the examples. Geometrical parameterization, shape optimization and integration in the CAD modeling for the ships and yachts design and analysis as well as geometrical reconstruction through biomedical data demonstrate the strength of the methods developed. As a last word, it looks even more promising, with the growth in knowledge and experience in the field of model order reduction, for computational scientists to be able to tackle more and more challenging problems.

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