An integrated data-driven computational pipeline with model order reduction for industrial and applied mathematics

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Abstract

In this work we present an integrated computational pipeline involving several model order reduction techniques for industrial and applied mathematics, as emerging technology for product and/or process design procedures. Its data-driven nature and its modularity allow an easy integration into existing pipelines. We describe a complete optimization framework with automated geometrical parameterization, reduction of the dimension of the parameter space, and nonintrusive model order reduction such as dynamic mode decomposition and proper orthogonal decomposition with interpolation. Moreover several industrial examples are illustrated.

1 Introduction

A very common problem in the optimization of the design of industrial artifacts is that of finding the shape that minimizes some quantity of interest representing the expected performance. From a mathematical point of view such a problem translates into an optimization problem in which a suitable algorithm makes several queries to a simulation solver allowing for an evaluation of each sample in the design space. This leads to the identification of the optimal solution, possibly subjected to a set of prescribed constraints.

The experience acquired through several industrial projects suggested us that for such pipeline to operate in a robust way in a manufacturing

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environment, several aspects have to be integrated and developed so as to deal with both complex geometries and solution fields. With the concept of digital twin becoming widespread nowadays, we have to be able to pass automatically from industrial CAD geometries to fluid dynamics and structural simulations which allow for virtual performance evaluation. All the steps in the procedure that, moving from a CAD geometry, leads to an optimized shape need to be carefully devised and integrated. First, one has to process the industrial geometry at hand through a suitable shape parameterization strategy which identifies the parameter space describing all possible designs to be investigated. After the generation of a suitable space including all the parameters that satisfy all the structural, geometrical, and regulatory constraints prescribed by the design engineers according to the stakeholders needs, a proper sampling of such space is used to set up a campaign of CFD and structural simulations resulting in the performance evaluation of each shape tested. Usually, a single full order industrial simulation takes days or even weeks, so it is crucial to develop reduced order models (ROMs) so as to speed up the full optimization cycle and make it compatible with the production needs. The computational time of a single sample point evaluation is reduced through different ROM techniques such as dynamic mode decomposition (DMD), and proper orthogonal decomposition (POD), both based on singular value decomposition [7, 8, 47, 45]. In the case of DMD, ROM is used to reconstruct and predict the spatiotemporal dynamics of a high fidelity simulation such that its evolution can be completed at a faster rate. Instead POD-Galerkin or POD with interpolation exploit data on previous simulations, properly stored, to provide accurate surrogate solutions corresponding to untested sample points in the parameter space. In such a way the computational cost of an online optimization cycle can be dropped to hours or even minutes.

In a further post-processing phase, we also apply a reduction of the parameter space exploiting the active subspaces property [12, 64, 62]. Such an analysis allows for the detection of possible redundancies in the chosen parameters, suggesting linear combinations of the original parameters which dominate the system response.

This work aims at presenting and discussing a series of best practice approaches for the application of each of the aforementioned techniques within an industrial optimization framework. Such approaches are the result of the constant involvement of mathLab laboratory of SISSA¹ in industrial projects joining the research efforts of both manufacturing companies and academic institutions. After a brief overview of the overall problem and goals, the contribution is arranged so as to present each of the described industrial numerical pipeline steps in a complete and detailed fashion. We first consider the geometrical treatment of the industrial artifacts shape, then we suggest

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possible parameter space reduction strategies. We then provide details on data-driven model order reduction methodologies, and finally present a brief summary of numerical results obtained in some applications carried out in the framework of industrial projects in which mathLab is involved.

2 From digital twin to real-time analysis

Nowadays the digital twin is a concept well spread among all the engineering companies and communities. With the exact digital representation of a physical system, it allows, for example, to perform structural and fluid dynamics simulations, to make sensitivity analysis with respect to the parameters, and to optimize the design. The increased number of devices for real-time data acquisition of the physical system makes the digital twin paradigm obsolete, due to its intrinsic static nature.

We are moving every day into a more dynamical representation of the entire system that takes into account more and more real-time data from different sources. This new paradigm, thanks to data-driven models, uncertainty quantification, machine learning algorithms, artificial intelligence and better integration of all the singular computational modules, will provide new capabilities in terms of discovery of hidden correlations, fault detection, predictive maintenance and design optimization. Its goal is to enable delivery of better simulation and modeling results, and thus shorter the product development, the so-called time-to-market, and reduce the product maintenance and potential downtime.

These new needs from the industrial point of view, lead to new mathematical methods and new interdisciplinary pipelines for data acquisition, model order reduction, data elaboration, as well as optimization cycles [4, 17, 25].

We can summarize a modern shape design optimization cycle with the diagram in Figure 1. Usually a CAD file describing the geometry to be optimized is provided by the design team, then we have the structural and CFD teams that provide physical constraints and admissible range for the parameters variation, we have data coming from the experiments on the scale model, and finally we have regulations constraints from the national authorities.

When the inputs of the simulation are set, the output is computed through high fidelity solver and the optimization cycle is closed by validation and control, the imposition of the constraints, and a selection of a new set of parameters. If a complete simulation takes several hours, even days, finding the optimal shape becomes impossible due to the many evaluations of the parametric PDE needed by the optimizer. Here, the model order reduction (MOR) approach allows fast evaluations of the output of interest

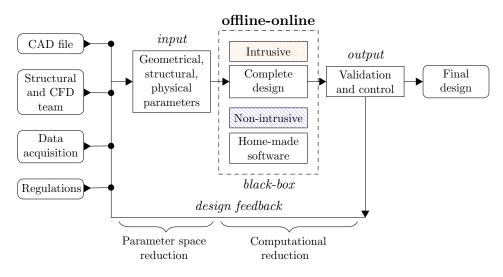


Figure 1: Complete optimization pipeline involving automatic interface with CAD files, experimental and numerical data acquisition, definition of the parameters constraints, and parameter space dimensionality reduction. Two possible reduced order methods are presented: an intrusive and a non-intrusive approach, allowing the creation of a complete simulation-based design optimization framework.

or derived quantities of the output thus enabling to find the optimum shape in few hours and to test different optimization algorithms. MOR techniques are very versatile, enabling both intrusive and non-intrusive approach with respect to the solver used. If it is a commercial black box it is possible to use numerical methods that work using only precomputed solution fields. While having access to the solver code allows also to reduce the single operators of the PDEs.

After the continued validation and control the optimization cycle ends by providing the final design in a suitable file format that can be analysed by all the interested departments.

In the following we are going to present all the techniques and integrated pipelines developed to accomplish such simulation based design optimization.

3 Advanced geometrical parametrization with automatic CAD files interface

The first important step is related to the geometry of the shapes considered. As previously mentioned, one of the aspects typically subjected to optimization in the design of industrial artifacts is in fact their geometry. Finding the shape by maximizing the performance of a certain product or of one of its components is in fact a very common problem in industry. From a mathematical standpoint, such class of problems is obviously formalized as an optimization problem, which consists in the identification of the point of a suitable parameter space that maximizes the value of a prescribed performance parameter (or output function). Although the mathematical algorithms carrying out such task are commonly well assessed, the mathematical formalization of the problem requires that the shape modification can be recast as the corresponding variation of a certain set of parameters. The latter operation, which somehow translates the properties of the geometrical shapes into a set of numbers handled by the optimization algorithms, is usually referred to as *shape parametrization*. In the most common practice the shape parametrization is a rather delicate part of the overall design process. In fact, as the shape to be studied can be specified in several different file formats or analytical descriptions, a unified approach for shape parametrization algorithms has currently not been established. In the present section we will describe and discuss the state of the art of shape parametrization techniques, and present examples of their application to the geometry of different industrial artifacts.

A first shape parametrization algorithm which has been devised so as to be applied to arbitrarily shaped geometries, is the free form deformation (FFD) [56, 36, 58]. FFD consists basically in three different steps, as depicted in Figure 2. The first step is that of mapping the physical domain into a reference one. In the second step, a lattice of points is built in such reference domain, and some points are moved to deform the lattice. Since the lattice points represent the control points of a series of shape functions (typically Bernstein polynomials), the displacement of such points is propagated to compute the deformation of all the points of the reference domain. In the third, final step, the deformed reference domain is mapped back into the physical one, to obtain the resulting morphed geometry.

So, the displacements of one or more of the control points in the lattice are the parameters of the FFD map, which is the composition of the three maps described. As both the number of points in the lattice and the number of control points displaced to generate the deformation are flexible, the FFD map can be built with an arbitrary number of parameters. Thus, a very useful feature of FFD, is that it allows for the generation of global deformations even when few parameters are considered.

Since FFD is able to define a displacement law for each point of the 3D space contained in the control points lattice, it can be quite naturally applied to all the geometries that are specified through surface triangulations, surface grids or even volumetric grids. As a first example, in Figure 3 we present the application of FFD to an STL triangulation, which is a very common output format for CAD modeling tools. The shape deformation illustrated in the picture has been carried out making use of the PyGeM [3]

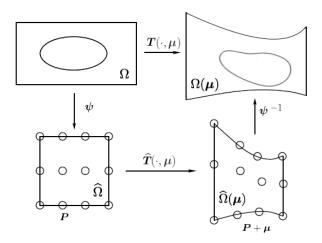


Figure 2: Sketch of the three maps composing the FFD map construction. ψ maps the physical space to the reference one, then \hat{T} deforms the entire geometry according to the displacements of the lattice control points, and finally ψ^{-1} maps back the reference domain to the original one.

Python package, which has been developed to be directly interfaced with the industrial geometry files and to deform them, so as to cut the communication times between the company simulation team and design team. In this application, the STL triangulation is imported and the coordinates of the nodes in the triangulation are modified according to the FFD map generated through the user specified lattice (included in the pictures).

The versatility of FFD can be further exploited to deform CAD surfaces that are generated as the collection of parametric patches. In such case, the desired deformation is obtained applying the specified FFD map to the control points of the NURBS and B-Splines surfaces of each patch composing the CAD model. The result in this case will also be a deformed geometry which follows the FFD deformation law specified by the user. Figure 4 presents a real world application of FFD to CAD parametric surfaces. The renderings show the original bulbous bow of the DTMB-5415 US Navy Combatant hull (which is a common benchmark for the CFD simulations community), and one of its several deformations generated to carry out the campaign of fluid dynamic simulations discussed in [18]. The PyGeM capabilities allow for importing the CAD geometry (in IGES or STEP format), extract and modify the control points of its surfaces and curves, and export the result into new CAD files.

Along with FFD, the PyGeM package implements other morphing techniques: the deformation based on radial basis function (RBF) interpolation [9, 40, 38], and the inverse distance weighting (IDW) interpolation [57,

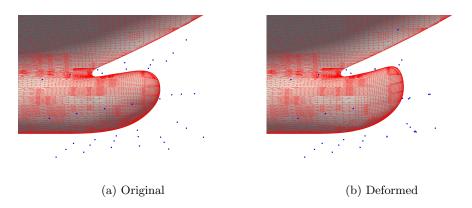
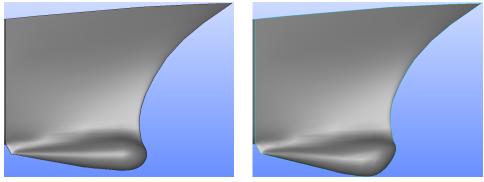


Figure 3: An example of the application of FFD to an STL triangulation. Plot (a) shows the FFD lattice over one side of the bulbous bow of a ship. Plot (b) depicts a deformed configuration of the same hull, along with the displaced FFD lattice control points.

67, 23, 5]. Yet, there are situations in which the shape to be deformed is already been engineered in a specific way, and general purpose deformation algorithms like FFD and the ones just mentioned would not preserve some critical characteristics of the geometry. A rather striking example of this is represented by the deformation of propeller blades illustrated in Figure 5. The shape of a propeller blade is in fact generated in a bottom-up fashion, first defining a set of sections represented by airfoils, and then properly placing each section in the three dimensional space. Since the aerodynamic feature of each airfoil section are known to the engineers which have selected them, any deformation that alters the sectional shape of the blade will not lead to an acceptable geometry. Thus, for such highly engineered shapes ad hoc solutions have to be generated. In most cases such solutions exploit the very algorithms used by the engineers to generate the artifacts in the first place, introducing parameters in one or more points of the generation procedure so as to create a class of deformed shapes. Also in this case, once the shape has been properly deformed (or re-generated), it has to be saved in the proper CAD format (IGES, STEP or STL) to be handled by the CFD or design team.

As mentioned, in the CAD data structures surfaces can be described both by means of a triangulation and as a collection of parametric patches. Yet, most CAD modeling tools used by engineers to generate the virtual model of any object designed, operate using NURBS and B-Splines curves and surfaces. On the other hand, several tools for CFD or structural analysis only handle geometries specified through triangulations. For such reason, a series of algorithms that generate triangulations on arbitrary parametric surfaces has been implemented in the last years. Among others, the ability



(a) Original

(b) Deformed

Figure 4: An example of the application of FFD to an IGES CAD geometry containing parametric surfaces. Plot (a) shows the original shape of the DTMB-5415 US Navy Combatant hull bulb. Plot (b) presents a deformed configuration of the same bulb.

to produce closed — or water tight — triangulations on surfaces composed of possibly unconnected faces is a crucial feature for both CFD and structural engineering applications. In fact, the neighboring parametric patches composing a CAD model are generally only connected up to a specified tolerance. Thus, it is not infrequent that ideally continuous surfaces present small gaps and overlaps between each patch composing them. To avoid the problem, most CAD modeling tools retain several logical information to complement the geometric data and indicate which patches should be considered as neighbors. Yet, converting to vendor-neutral file formats such as IGES of STEP that allow the digital exchange of information among CAD systems will cause in most case the loss of topological information on neighboring patches. This is often a problem in the numerical analysis community, in which geometries are in most cases obtained by third parties, and in which water tight surfaces are in needed to define (and confine) the three dimensional domains considered in the simulations. So, a possible strategy to avoid a surface triangulation that depends on the local patches parametrization, and suffers from parametrization jumps and gaps, is to create new nodes not in the surface parametric space, but in the physical three dimensional space. Since such new nodes will not be initially located onto the CAD surface, a series of surface and curves projectors are used to make sure that the new grid points are properly placed onto the surface in a way that is completely independent of the parametrization. Along with the projectors, presented in [16], the work in [39] describes an algorithm which allows for the hierarchical refinement of an initial blocking made of quadrilateral cells. Across each level of refinement, the cells located in the highest curvature regions are refined, until a prescribed accuracy is reached.

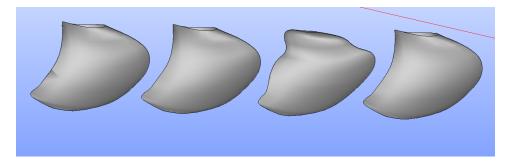


Figure 5: An example of the deformation of an engineered propeller blade shape. The picture shows four deformed configurations of a PPTC benchmark propeller blade, in which the sectional properties of the blade have been kept untouched, while modifying the pitch, rake and skew distributions. The deformations are performed with the BladeX Python package [2].

Figure 6 shows the geometry (left side) and quadrilateral grid generated on a planing yacht hull. As can be appreciated, the grid is consistently refined in the high curvature regions located around the double chine line, and on the spray rails. Finally, once this quadrilateral water tight mesh is obtained, the cells are split into triangles to obtain a water tight STL triangulation, which can be an ideal input for numerical analysis software.



Figure 6: Water tight quadrilateral mesh generated on the water non tight IGES surface of a planing yacht hull.

We remark that all the presented applications exemplify the employment of the numerical pipeline proposed in the framework of the industrial POR-FESR projects SOPHYA "Seakeeping Of Planing Hull YAchts", PRELICA "Advanced methodologies for hydro-acoustic design of naval propulsion", and FSE HEaD "Higher Education and Development" programme founded by European Social Fund, in which mathLab laboratory has been involved in the last years.

4 Parameter space dimensionality reduction

After all the contributions from the different teams, the number of parameters could be too big for a reasonable optimization cycle in terms of computational time. In other cases, even if the parameters are not too many, there could be some of them dependent on the others. To overcome this problem it is possible to reduce the dimensionality of the parameter space by finding an active subspace (AS) [12] of the target functions. This technique ascertains whether the output of interest can be approximated by a function depending by linear combinations of all the original parameters. Its application has been proven successful in several parametrized engineering models [26, 13, 18, 64].

Now we briefly review the process of finding active subspaces of a scalar function f representing the output of interest, and depending on the inputs $\mu \in \mathbb{R}^m$. Let us assume $f : \mathbb{R}^m \to \mathbb{R}$ is a scalar function continuous and differentiable in the support of a probability density function $\rho : \mathbb{R}^m \to \mathbb{R}^+$. We assume f with continuous and square-integrable (with respect to the measure induced by ρ) derivatives. We define the active subspaces of the pair (f, ρ) as the eigenspaces of the covariance matrix associated to the gradients $\nabla_{\mu} f$. The elements of this matrix, the so-called uncentered covariance matrix of the gradients of f, denoted by \mathbf{C} , are the average products of partial derivatives of the simulations' input/output map, i.e.:

$$\mathbf{C} = \mathbb{E}\left[\nabla_{\boldsymbol{\mu}} f \,\nabla_{\boldsymbol{\mu}} f^T\right] = \int_{\mathbb{D}} (\nabla_{\boldsymbol{\mu}} f) (\nabla_{\boldsymbol{\mu}} f)^T \rho \, d\boldsymbol{\mu},$$

where $\mathbb{E}[\cdot]$ is the expected value. The matrix **C** is symmetric and positive semidefinite, so it admits a real eigenvalue decomposition $\mathbf{C} = \mathbf{W} \mathbf{\Lambda} \mathbf{W}^T$, where **W** is a $m \times m$ orthogonal matrix of eigenvectors, and $\mathbf{\Lambda}$ is the diagonal matrix of the eigenvalues, which are non-negative, arranged in descending order.

Now we select the first M eigenvectors, for some M < m, forming a lower dimensional parameter subspace. We underline that, on average, low eigenvalues suggest the corresponding vector is in the nullspace of the covariance matrix. So we can construct an approximation of f by taking the eigenvectors corresponding to the most energetic eigenvalues. Let us partition Λ and \mathbf{W} as follows:

$$oldsymbol{\Lambda} = egin{bmatrix} oldsymbol{\Lambda}_1 & \ & oldsymbol{\Lambda}_2 \end{bmatrix}, \qquad oldsymbol{W} = egin{bmatrix} oldsymbol{W}_1 & oldsymbol{W}_2 \end{bmatrix},$$

where $\Lambda_1 = \text{diag}(\lambda_1, \dots, \lambda_M)$, and \mathbf{W}_1 contains the first M eigenvectors. The range of \mathbf{W}_1 is the active subspace, while the inactive subspace is the range of \mathbf{W}_2 . By projecting the full parameter space onto the active subspace we approximate the behaviour of the target function with respect to the new reduced parameters.

The active variable μ_M , and the inactive one η , are obtained from the input parameters as follows:

$$\boldsymbol{\mu}_M = \mathbf{W}_1^T \boldsymbol{\mu} \in \mathbb{R}^M, \qquad \boldsymbol{\eta} = \mathbf{W}_2^T \boldsymbol{\mu} \in \mathbb{R}^{m-M}.$$

That means that we can express any point in the parameter space $\mu \in \mathbb{R}^m$ in terms of μ_M and η as:

$$oldsymbol{\mu} = \mathbf{W}\mathbf{W}^Toldsymbol{\mu} = \mathbf{W}_1\mathbf{W}_1^Toldsymbol{\mu} + \mathbf{W}_2\mathbf{W}_2^Toldsymbol{\mu} = \mathbf{W}_1oldsymbol{\mu}_M + \mathbf{W}_2oldsymbol{\eta}.$$

So we can rewrite f as $f(\boldsymbol{\mu}) = f(\mathbf{W}_1 \boldsymbol{\mu}_M + \mathbf{W}_2 \boldsymbol{\eta})$, and construct a surrogate quantity of interest g using only the active variable $\boldsymbol{\mu}_M$

$$f(\boldsymbol{\mu}) \approx g(\mathbf{W}_1^T \boldsymbol{\mu}) = g(\boldsymbol{\mu}_M).$$

Active subspaces can also be seen in the more general context of ridge approximation [14, 42, 33].

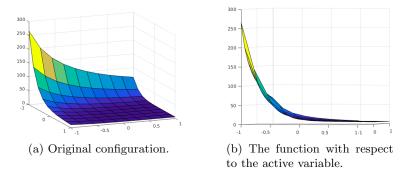


Figure 7: Example of a scalar output function depending on two parameters. After a proper rotation of the whole domain it is possible to highlight the behaviour of the quantity of interest along the active direction.

From a practical point of view, expressing a target function with respect to its active variable means to rescale the parameter space on the origin and then rotate it so as to unveil the low rank behaviour of the function. In Figure 7 an example involving a bivariate scalar function is depicted. This approach can be viewed as a preprocessing step in the optimization cycle that helps both in reducing the number of the parameters and to increase the accuracy of a further reduction of the model as proven in [62] for the computation of the pressure drop in an occluded carotid artery using active subspace and POD-Galerkin methods. Other approaches focus only on the shape parameters. To retain a significant geometric variance while reducing the number of geometrical parameters there exist nonlinear methods such as, among others, Kernel PCA [54, 55], Local PCA [32], and particular neural network such as Auto Encoders and Deep Auto Encoders [31]. For a comprehensive comparison among them we refer to [15], where the methods are demonstrated for the design-space dimensionality reduction of a destroyer hull. For a comparison between 13 different nonlinear techniques see [66].

5 Data driven model order reduction

In the *big data* era, data-driven models is becoming more and more popular in order to extract as much information as possible from all the data acquired during the physical experiments and the simulations. We mention also *uncertainty quantification* and ROM algorithms modified "ad hoc" [11]. Also in model order reduction community, several techniques have been developed to face industrial problems with a non-intrusive approach.

5.1 Dynamic mode decomposition

Dynamic mode decomposition (DMD) has emerged as a powerful tool for analyzing the dynamics of nonlinear systems, and for postprocessing spatiotemporal data in fluid mechanics [52, 53, 61]. It was developed by Schmid in [51], and it is an equation-free algorithm, and it does not make any assumptions about the underlying system. DMD allows to describe a nonlinear time-dependent system as linear combination of few main structures evolving linearly in time. Many variants of the DMD were developed in the last years like forward backward DMD, compressed DMD [21], multiresolution DMD [35], higher order DMD [37], and DMD with control [43] among others. For a complete review refer to [34, 65], while for an implementation of them we refer to the Python package called PyDMD [20]. Lots of these variants arose to solve particular industrial problems such as streaming DMD [27] that are able to feed the classical algorithm with new real-time data coming from sensors, and do not require storage of past data, and they prove useful for real-time PIV or smoke/dye visualizations. In presence of very large dataset for complex industrial model the DMD modes are computed via randomized methods [22]. We cite also a new paradigm for data-driven modeling that simultaneously learns the dynamics and estimates the measurement noise at each observation that uses deep learning and DMD for signal-noise decomposition [46].

Now we present a brief overview of the standard algorithm. Let us consider *m* vectors, equispaced in time, representing the state of our system, also called *snapshots*: $\{\boldsymbol{x}_i\}_{i=1}^m$. The idea is that there exists a linear operator **A** that approximates the nonlinear dynamics of $\boldsymbol{x}(t)$, i.e. $\boldsymbol{x}_{k+1} = \mathbf{A}\boldsymbol{x}_k$.

Without explicitly computing the operator \mathbf{A} we seek to approximate its eigenvectors and eigenvalues, and we call them DMD modes and eigenvalues. First of all we arrange the snapshots in two matrices \mathbf{X} and \mathbf{Y} so as each column of the latter contains the state vector at the next timestep of the one in the corresponding \mathbf{X} column, as follows

$$\mathbf{X} = \begin{bmatrix} x_1^1 & x_2^1 & \cdots & x_{m-1}^1 \\ x_1^2 & x_2^2 & \cdots & x_{m-1}^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^n & x_2^n & \cdots & x_{m-1}^n \end{bmatrix}, \qquad \mathbf{Y} = \begin{bmatrix} x_2^1 & x_3^1 & \cdots & x_m^1 \\ x_2^2 & x_3^2 & \cdots & x_m^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_2^n & x_3^n & \cdots & x_m^n \end{bmatrix}.$$

We are looking for **A** such that $\mathbf{Y} \approx \mathbf{A}\mathbf{X}$. The best-fit **A** matrix is given by $\mathbf{A} = \mathbf{Y}\mathbf{X}^{\dagger}$, where the symbol † represents the Moore-Penrose pseudo-inverse.

The DMD algorithm projects the data onto a low-rank subspace defined by the POD modes, that are the first r left-singular vectors of the matrix \mathbf{X} . We compute them via truncated singular value decomposition as $\mathbf{X} \approx \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^*$. The unitary matrix \mathbf{U}_r contains the first r modes. So we can express the reduced operator $\tilde{\mathbf{A}} \in \mathbb{C}^{r \times r}$ as

$$ilde{\mathbf{A}} = \mathbf{U}_r^* \mathbf{A} \mathbf{U}_r = \mathbf{U}_r^* \mathbf{Y} \mathbf{X}^\dagger \mathbf{U}_r = \mathbf{U}_r^* \mathbf{Y} \mathbf{V}_r \mathbf{\Sigma}_r^{-1} \mathbf{U}_r^* \mathbf{U}_r = \mathbf{U}_r^* \mathbf{Y} \mathbf{V}_r \mathbf{\Sigma}_r^{-1},$$

avoiding the computation of the high-dimensional operator **A**. $\tilde{\mathbf{A}}$ defines the linear evolution of the low-dimensional model $\tilde{\boldsymbol{x}}_{k+1} = \tilde{\mathbf{A}}\tilde{\boldsymbol{x}}_k$, where $\tilde{\boldsymbol{x}}_k \in \mathbb{R}^r$ is the low-rank approximated state. The high-dimensional state \boldsymbol{x}_k can then be easily computed as $\boldsymbol{x}_k = \mathbf{U}_r \tilde{\boldsymbol{x}}_k$.

Exploiting the eigendecomposition of $\tilde{\mathbf{A}}$, that is $\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\mathbf{\Lambda}$, we can reconstruct the eigenvectors and eigenvalues of the matrix \mathbf{A} . The elements in $\mathbf{\Lambda}$ correspond to the nonzero eigenvalues of \mathbf{A} , while the eigenvectors of \mathbf{A} can be computed in two ways. The first one is by projecting the low-rank approximation \mathbf{W} on the high-dimensional space: $\mathbf{\Phi} = \mathbf{U}_r \mathbf{W}$. We call the eigenvectors $\mathbf{\Phi}$ the *projected* DMD modes. The other possibility is the so called *exact* DMD modes [65], that are the real eigenvectors of \mathbf{A} , and are computed as $\mathbf{\Phi} = \mathbf{Y} \mathbf{V}_r \boldsymbol{\Sigma}_r^{-1} \mathbf{W}$.

DMD has also been successfully used to accelerate the computation of the total drag resistance of a hull advancing in calm water [63, 17, 18]. This responded to the industrial needs of a rapid creation of the offline dataset. We decided not only to identify the approximated dynamics of the system but also to predict its evolution in order to achieve the regime state using only few snapshots, as we show in the example reported in Figure 8.

5.2 Proper orthogonal decomposition with interpolation

Proper orthogonal decomposition with interpolation (PODI) is an equationfree model order reduction technique providing a fast approximation of the



Figure 8: Example of DMD application for wall shear stress prevision. In the top image, we show the wall shear stress along the x direction, at time t = 50s, computed using full-order solver. In the bottom, we show the wall shear stress along x direction reconstructed at time t = 50s using 30 snapshots equispaced in the temporal window [1, 30].

solution of a parametric PDE. The key idea is to approximate the solution manifold by interpolating a finite set of high-fidelity snapshots, computed for some chosen parameters. Since interpolation of high dimensional data can be very expensive, we need reduced order modelling for a real-time evaluation of the solution for the new parameters.

This method consists in two logical phases: in the *offline* one, the high-fidelity solutions of a finite set of deformed configurations are computed and stored into the matrix \mathbf{S} such that:

$$\mathbf{S} = \begin{bmatrix} s_1 & s_2 & \dots & s_m \end{bmatrix}, \quad s_i \in \mathbb{R}^n \quad \text{for } i = 1, 2, \dots, m.$$

The basis spanning the low dimensional space is computed applying the singular value decomposition on the snapshots matrix:

$\mathbf{S}=\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{*},$

where $\mathbf{U} \in \mathbb{C}^{n \times m}$ refers to the matrix whose columns are the left singular vectors — the so called *POD modes* — of the snapshots matrix. We project the high-fidelity solutions onto the low-rank space, so they are represented as linear combination of the modes and the coefficients of this combination are called modal coefficients.

In the *online* phase the modal coefficients are interpolated and finally, for any new parameter, the solution of the parametric PDE is approximated. This method has the great benefit of being based only on the system output, but the accuracy of the approximation depends on the chosen interpolation method. The algorithm has been implemented in an open source Python package called EZyRB [19]. For deeper details about the PODI, we recommend [49, 10, 44].

6 Simulation-based design optimization framework

As previously stated, a shape optimization pipeline is usually composed by three fundamental ingredients: a deformation technique to construct the set of admissible shape, an objective function, and an optimal strategy to converge to the optimal shape with the lowest number of evaluations. Depending on the studied physical phenomena, the entire process can be very long: many complex problems, as for example conductivity, diffusion and fluid dynamic, are described through partial differential equations (PDEs). The numerical solution of such equations is usually expensive from the computational viewpoint. Moreover, in an optimization scenario, these equations have to be solved at each iteration, making the computational cost unaffordable for many applications, especially in the industrial sectors where a high responsiveness is requested to reduce the time-to-market. The model order reduction (MOR) offers the possibility to efficiently compute the solution of parametric PDEs, drastically reducing the computational effort. We exploited MOR techniques to design an innovative shape optimization pipeline which fits the industrial needs, primarily in terms of efficiency, reliability and modularity. The key idea of this optimization procedure is to collect the solutions, or the output of interest, from the full-order model for a finite set of parameters, then combining these solutions for a fast evaluation of the solution for any new iteration of the optimization algorithm.

In the first step, the deformed shapes are created from the initial geometry by using a combination of parameters. There are many possible techniques to choose from, as presented in Section 3. The important aspect is that given a set of parameters, the software is able to generate a new deformed geometry.

The parameter space is sampled and the system configurations so-created are evaluated using the high-fidelity numerical method. The pipeline relies only on the system outputs, without requiring information about the physical system, making all the procedure independent from the high-fidelity solver. Especially in an industrial context, this guarantees a great plus, allowing to adopt any solver — also commercial — within the pipeline. Further, the non-intrusive approach preserves the industrial know-how and reduces the complexity in the implementation phase.

We use two different data-driven model order reduction methods to accelerate the optimization. With the dynamic mode decomposition described in Section 5.1 we can simulate the physical problem at hand for a shorter temporal window using the computational expensive full-order solver and apply the DMD on the produced output to predict the solution/output of interest at regime. The second model order reduction technique adopted in the pipeline is the PODI, discusses in Section 5.2. Thanks to this method, we have the possibility to approximate in a real-time context the solution of parametric PDEs, combining several pre-computed snapshots. We adopt

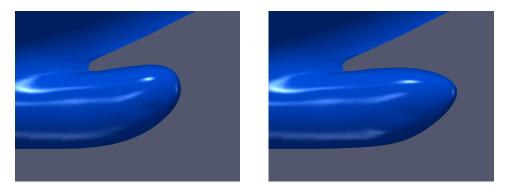


Figure 9: Example of the shape optimization pipeline applied on naval hull: the original shape (left) and the optimized shape (right).

PODI in order to deal only with the output data of the high-fidelity solver, thus let the pipeline be independent from the used full-order model. To increase the accuracy of the reduced order model, an intrusive approach can be adopted. For an exhaustive discussion on the intrusive model order reduction, we suggest [59, 60] due to the implementation of MOR methods in a finite volume (FV) framework, the nowadays industrial standard for many fluid dynamics applications. For an overview on projection-based ROMs and the effort in increasing the Reynolds number see [29, 6], and for the joint use of such methods and uncertainty quantification strategies based on non intrusive polynomial chaos see [30]. Another possibility is to link together the isogeometric analysis with MOR into a complete parametric design pipeline from CAD to accurate and efficient numerical simulation [48, 24]. For a complete discussion about ROM for parametric PDEs, we recommend [28].

The optimization algorithm relies so on the reduced order model: since the online phase returns the approximated solutions in a quasi real-time scenario, the optimization algorithm lasts minutes or hours to reach the optimal shape, also if thousands of iterations are needed. The computational cost of the procedure is due to the creation of the solutions database. Thanks to MOR, we have also the possibility to run and tests many different optimization algorithms, avoiding any further high-fidelity simulations. Moreover, the solutions database can be enriched to increase the accuracy of the reduced order model. Examples of optimization procedure involving MOR techniques applied into naval and aerodynamics fields are respectively [17, 50]. Figure 9 shows the results of the application of the shape optimization system on the bulbous bow of a cruise ship. This achievement has been developed in the framework of a regional European Social Fund project from Regione Friuli Venezia-Giulia: HEaD in collaboration with Fincantieri - Cantieri Navali Italiani S.p.A..

7 Conclusions and perspectives

Industrial computational needs are every day more and more demanding in terms of computational time, reliability, error certification, data-assimilation, robustness, and easiness of use. In this work we presented several model order reduction and shape parameterization techniques to solve industrial and applied mathematics problems.

More has to be made to integrate real-time data-assimilation, machine learning and prediction, but we are moving along this horizon and MOR will play a crucial role to tackle many complexities arising from complex industrial artifacts management. A step in this direction is the planned webserver ARGOS [1], developed by mathLab group at SISSA that will make possible the exploitation of reduced order models to a vast category of people working in design, structural, and CFD teams. Through specific web applications the user will be able to solve many industrial and biomedical problems without the need of being an expert in numerical analysis and scientific computing. Figure 10 depicts some of the possible applications that are currently being developed.

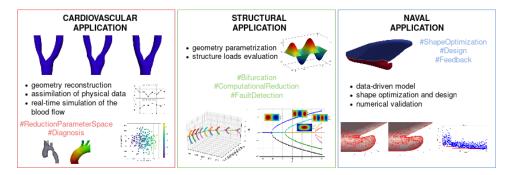


Figure 10: Possible extension of the presented pipeline with different goal and application fields. From cardiovascular problems like real-time blood flow simulation, to structure load analysis and identification, as well as naval applications.

We also cite the Artificial Student "Artie" [41] that accepts problem statements posed in natural language, and solves numerically some PDEs problems, that will help both students, the scientific staff, and engineers in general. Moreover we want to highlight the effort of the Italian government in the technology transfer thanks to the institution of several competence centers connecting research facilities, university, and companies in the framework of Industry 4.0. Similar initiatives are undergoing in many other European countries (France, Germany, UK, ...).

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