The medical digital twin assisted by Reduced Order Models and Mesh Morphing

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Summary

Nowadays silico analysis tools in the bio-medical field are moving from the research context to the patient specific treatment and prevention one. Hemo-dynamics is receiving a great attention and an accurate CFD modelling can be adopted to produce a digital medical twin capable to reliably predict pathology the evolution and the effect of surgical corrections. The availability of in silico digital twins based on CAE simulations is one of the key enablers; parametric shape of vessels and reduced order models (ROM) are a promising solution. The ROM approach requires HPC to be built, but it can be consumed almost in real time and outside from the standard CAE tools as well. In this paper the concept is demonstrated exploiting the new ROM Builder available in ANSYS 19.1. We developed a pipeline for the aortic aneurysm to study the effect of the bulge shape progression on the flow field. First a patient-specific geometry was reconstructed, then a CFD model was created with a bulge shape parameterised through an RBF mesh morphing technique. Finally, a ROM was suitably built up carrying out CFD simulations. Examples of fast evaluations achieved off-line by consuming ROM results are provided.

Keywords

Digital Twin, Reduced Order Model, CFD, RBF, mesh morphing, CVDs

Introduction

Cardiovascular diseases (CVDs) are the main cause of death in the world, resulting in 17.9 million deaths (32.1%) in 2015 only [1]. It is estimated that up to 90% of this casualties can be predicted and prevented [2]. In silico analysis can help in this regard, improving these figures by preventing and analysing patient-specific tailored systems. The evolution and growing availability of computational power has extended this concept by enabling the employment of high fidelity CAE simulations and the development of medical digital twins, able to provide a safe environment in which the pathology evolution can be predicted and the impact of potential surgical corrections explored. For CVD pathologies the hemo-dynamic of the vessels can be thoroughly examined by recurring to high fidelity computational fluid dynamics (CFD) techniques and tools. The large number of degrees of freedom present in a real clinical case, however, make this approach computationally expensive and not directly suitable to test a patient-specific case virtually and in real-time. Several methodologies such as stochastic approaches for geometrical variations, material properties and uncertainty quantification [3][4][5], have been developed and are available in literature to overcome this problem. However, none of them is able to cope with the full field of variable of interest, thus providing quantitative output in real time. In this regard ROM are emerging as a viable technology able to provide complex multi degree of freedom full-scale solutions drastically reducing the overall computing cost. While the use of ROM systems is well-known and has received significant attention in the last decade, its use is mainly limited to classical mechanics [6] and dynamics [7], and their implementation in the field of biomechanics is very recent and limited to few works [8]. The ROM ability to investigate the effect of a huge number of parameters in real-time can be synergistically combined with the properties of mesh-morphing techniques, able to provide the huge number of geometrical variations. Radial Basis Functions (RBF) [9] have been demonstrated to be a powerful morphing tool in several fields, including the medical one [10].

In this paper a workflow envisioning the use of the ROM implementation available in ANSYS 19.1 and the commercial morpher RBF Morph is proposed and applied to the investigation of the hemodynamic field for a wide set of ascending thoracic aneurysmatic aortic (aTAA) morphologies. In the next section the background on ROM and RBF will be briefly given. The proposed workflow will be then introduced and demonstrated for the accomplishment of a test-case dealing with an ATAA case.

ROM and RBF Background

ROM

Model Reduction is a technique that allows a cost-efficient evaluation of large degree of freedom (DOF) systems by reducing the number of variables involved in the problem. This simplification, while preserving the essential characteristics of the system enabling an accurate and efficient representation, makes feasible a real-time control over the parameters of the problem. ROM have been successfully applied during the years to controls [11], fluid dynamics, structural dynamics, thermal analysis, multi-physics [12], medical [13] and optimization problems [14]. Several techniques to obtain a ROM representation have been explored and are available in literature to the scientific community. The one employed in this paper is based on the Proper Order Decomposition (POD) technique and is implemented as a commercial software in ANSYS Workbench 19.1 [15]. A typical workflow including the use of ROM, shown in figure 1, is composed by two main tasks typically referred to as creation and consumption. The first deals with all the processes needed to generate and extract the information from the full DOF system, namely the training of the ROM using a simulation software and the extraction of the most important modes using a POD technique. The latter concerns the use of such extracted modes to produce a reduced order system in real time. This task can be accomplished either employing the ANSYS ROM viewer, that is a standalone software designated to ROM consumption, or importing the reduced system into ANSYS Fluent.

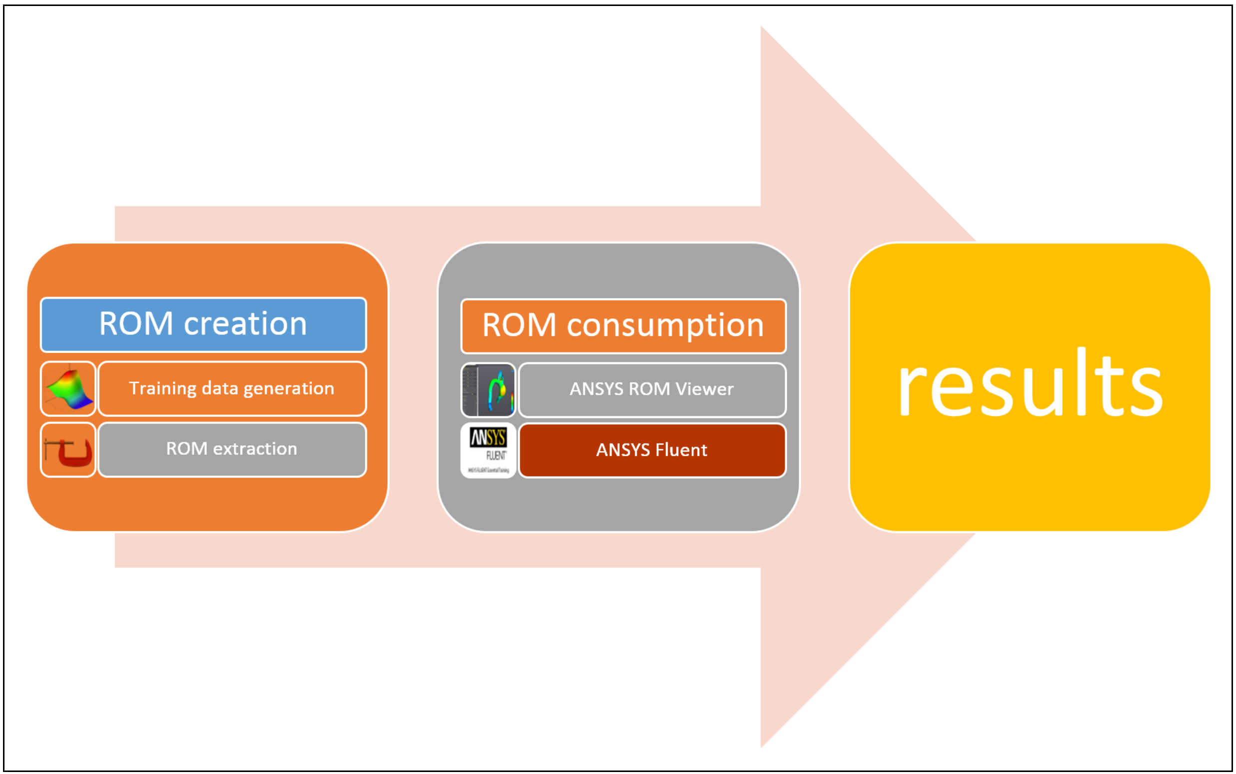

Figure 1: ANSYS ROM usage workflow

Being the reduced system a direct consequence of the input parameters variation and generation of a number of Design Points (DP), the ROM environment implemented by ANSYS is designed to be strongly intertwined with the concept of Response Surface (RS). The training data generation is indeed produced by evaluating, at full scale, a given number of DP called snapshots. The higher the number of snapshots, the more faithful the reduced order model, thus catching all the nuances of the system produced by a parameter variation. The quality of the reduced model is also influenced by the number of modes employed for its discretization. In ANSYS Workbench the result of the ROM creation task can be saved as a standalone file that includes the reduced system and the numerical grid of the problem. When needed this file can be then imported into the consumption task by exploiting the standalone ANSYS ROM viewer or, instead, loaded into ANSYS Fluent as an alternative of the *.cas and *.dat files.

RBF background

From mathematical point of view, the solution of the RBF problem consists of the calculation of the coefficients of a linear system of order equal to the number source points (De Boer et al., 2007), by means of which the displacement of an arbitrary mesh's node (target) can be expressed, and then imposed, as the summation of the radial contribution of each controlled node (source). In such a way, mesh smoothing can be rapidly applied by maintaining mesh topology in terms of total number and type of elements.

In particular, the RBF Morph tool utilizes the RBF interpolant $\boldsymbol{s}$ composed by a radial function containing the RBF φ and a multivariate polynomial corrector vector h of order $m-1$, where m is said to be the order of φ, introduced with the aim to assure the uniqueness of the RBF solution and the compatibility for rigid motions. Specifically, if N is the total number of source points, the formulation of the RBF interpolant is

$$s(\boldsymbol{x}) = \sum \boldsymbol{\gamma_i}\varphi(\|\boldsymbol{x} - \boldsymbol{x_{k_i}}\|) + h(\boldsymbol{x}) \tag{1}$$

where $\boldsymbol{x}$ is the vector identifying the position of a generic node belonging to the surface and/or volume mesh $\boldsymbol{x_{k_i}}$ is the ith source node position vector and ||·|| is the Euclidean norm.

The RBF fitting solution exists in case the RBF coefficients vector $\boldsymbol{\gamma}_i$ and the weights of the polynomial corrector vector $\boldsymbol{\beta}_i$ can be found such that, at source points, the interpolant function possesses the specified (known) values of displacement $\boldsymbol{g}_i$, whilst the polynomial terms give a null contribution, namely the following relations are simultaneously verified

$$s(\boldsymbol{x_{k_i}}) = \boldsymbol{g_i} \qquad 1 \le i \le N \tag{2}$$

$$\sum \boldsymbol{\gamma}_i q(\boldsymbol{x_{k_i}}) = 0 \tag{3}$$

for all polynomials q with a degree less than or equal to that of polynomial h (Beckert and Wendland, 2001). The minimal degree of polynomial h depends on the choice of the RBF type. It can be demonstrated that a unique RBF interpolant exists if the RBF is conditionally positive definite (Van Zuijlen et al., 2007). In the case that this latter condition is established and if the order is less than or equal to 2 (Jin et al., 2001), a linear polynomial applies

$$h(\boldsymbol{x}) = \boldsymbol{\beta_1} + \boldsymbol{\beta_2}x + \boldsymbol{\beta_3}y + \boldsymbol{\beta_4}z \tag{4}$$

enabling to exactly recover rigid body translations.

In the event such assumptions are verified, the interpolant has the form

$$s(\boldsymbol{x}) = \sum \boldsymbol{\gamma}_i \varphi(\|\boldsymbol{x} - \boldsymbol{x}_{\boldsymbol{k}_i}\|) + \boldsymbol{\beta}_1 + \boldsymbol{\beta}_2 x + \boldsymbol{\beta}_3 y + \boldsymbol{\beta}_4 z \quad (5)$$

and $\boldsymbol{\gamma}_i$ and $\boldsymbol{\beta}_i$ values can be obtained by solving the system

$$\begin{pmatrix} \boldsymbol{U} & \boldsymbol{P} \\ \boldsymbol{P}^T & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\beta} \end{pmatrix} = \begin{pmatrix} \boldsymbol{g} \\ \boldsymbol{0} \end{pmatrix} \quad (6)$$

where $\boldsymbol{U}$ is the interpolation matrix having the elements derived by calculating all the radial interactions between source points as follows

$$U_{ij} = \varphi\left(\left\|\boldsymbol{x}_{\boldsymbol{k}_i} - \boldsymbol{x}_{\boldsymbol{k}_j}\right\|\right) \qquad 1 \le i \le N, \qquad 1 \le j \le N \quad (7)$$

and $\boldsymbol{P}$ is a constraint matrix that arises balancing the polynomial contribution, that is

$$\boldsymbol{P} = \begin{pmatrix} 1 & x_{k_2} & y_{k_2} & z_{k_2} \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \quad (8)$$

assuming that source points are not contained in the same plane (otherwise the interpolation matrix would be singular).

For what described, by satisfying the displacement field prescribed at source points, RBF Morph operates the smoothing of mesh nodes using the following formulation of the interpolant

$$\begin{cases} s_y(\boldsymbol{x}) = \sum \gamma_i^y \varphi(\|\boldsymbol{x} - \boldsymbol{x}_{\boldsymbol{k}_i}\|) + \beta_1^y + \beta_2^y x + \beta_3^y y + \beta_4^y z \end{cases} \quad (9)$$

A great flexibility using RBF can be achieved acting on the radial functions that can be compactly or globally supported. Common options are summarized in table 1**Errore. L'origine riferimento non è stata trovata.**. RBF Morph allows 4 radial functions. The distance function (global supported and bi-harmonic in 3D) is used by default and performs very well in volume morphing as it allows to get very good quality and it is accelerated so that it can handle RBF problem beyond 1 million of centres (source points). Wendland functions (C0,C2 and C4) are available for surface sculpting as the high level of continuity can be used to control a surface using just a few control points.

Radial Basis Functions (RBF) with global support	$\varphi(r)$
Spline type (Rn)	$r^n, n\ odd$
Thin plate spline (TPSn)	$r^n \log(r), n\ even$
Multiquadric (MQ)	$\sqrt{1+r^2}$
Inverse multiquadric (IMQ)	$\frac{1}{\sqrt{1+r^2}}$
Inverse quadratic (IQ)	$\frac{1}{1+r^2}$
Gaussian (GS)	e^{-r^2}
Radial Basis Functions (RBF) with compact support	$\varphi(r) = f(\xi), \xi \le 1, \xi = \frac{r}{R_{sup}}$

Radial Basis Functions (RBF) with global support	$\varphi(r)$
Wendland C0 (C0)	$(1-\xi)^2$
Wendland C2 (C2)	$(1-\xi)^4(4\xi+1)$
Wendland C4 (C4)	$(1-\xi)^6\left(\frac{35}{3}\xi^2+6\xi+1\right)$

Table1: Typical RBF

Application Description

The application selected to describe the proposed workflow is an ascending aorta aneurysm. In the following sections the information regarding ROM and RBF setup is detailed.

CFD models generation

The geometry taken into account and its shape variations are the result of a processing of data pertaining to an aneurysmatic aorta SSGA, defined according to the procedure described in Capellini et al. [16]. The 3D model was obtained as a result of a statistical analysis of aortic morphological shapes of 45 aneurysmatic patients (Fig.2a) whose CT datasets were retrospectively segmented and elaborated by VMTK software and Python custom scripts. The SSGA model was parameterized to create a CFD model able to cope with a large number of ascending aneurysmatic aortic configurations through shape deformations. Three of the parameters evaluated in the previous work statistical analysis were considered to follow the bulge variations: the maximum diameter of the aneurysm (D_{max}), the tortuosity value (T) of the centreline of ascending portion of aorta and the bulge extension (B_{ext}). These parameters were assumed to vary in specific intervals extracted from the results of statistical analysis reported in Capellini et al. [16]. In particular, a range of an average value ± standard deviation was considered for each parameter (D_{max} = [45.69-55.95 mm], T= [0.0776-0.1484], B_{ext} = [17.93-41.69 mm]). In figure 2(b) the SSGA model including the ascending centreline, the D_{max} and the B_{ext} are depicted.

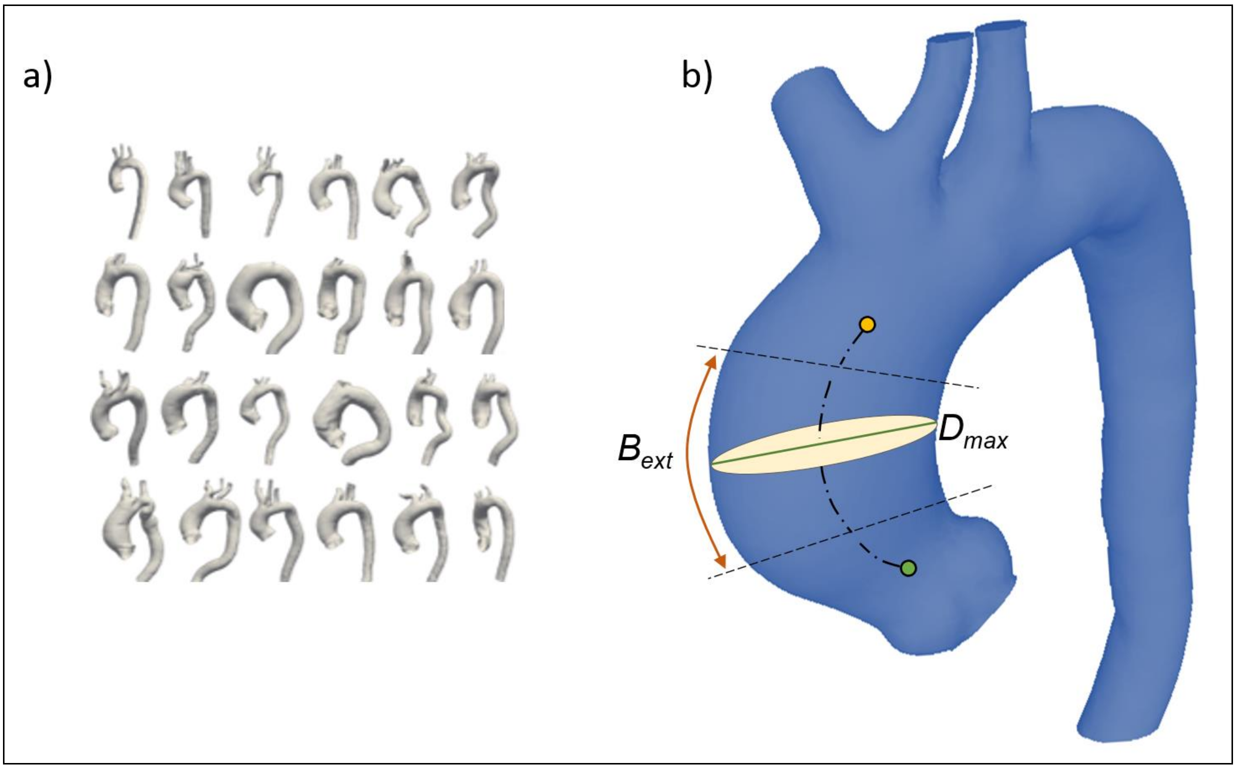

Figure 2: Statistical aneurysmatic aorta

RBF set-up

The mesh morphing action was accomplished using the commercial morpher RBF Morph. A set of source points on the ascending thoracic aortic region was selected to generate 5 shape variations representative of the statistic geometry explained in the previous section. In figure 3 the RBF setup is shown. Three sets of RBF points were generated as shown in figure 3a, maintaining fixed the extremal sets (green and red in the picture) in order to circumscribe the morphing action. The central set was translated in the plane over which the points were defined (figure 3b, 3c and 3d), and scaled over the same plane along the principal directions (figure 3e and 3f). This set of 5 shapes modifications was chosen in order to generate the representative variations shown in figure 2a. The time required to morph the 1.5 million elements tetrahedral CFD mesh for each DP was 43s on an i7 laptop with 16 GB of RAM.

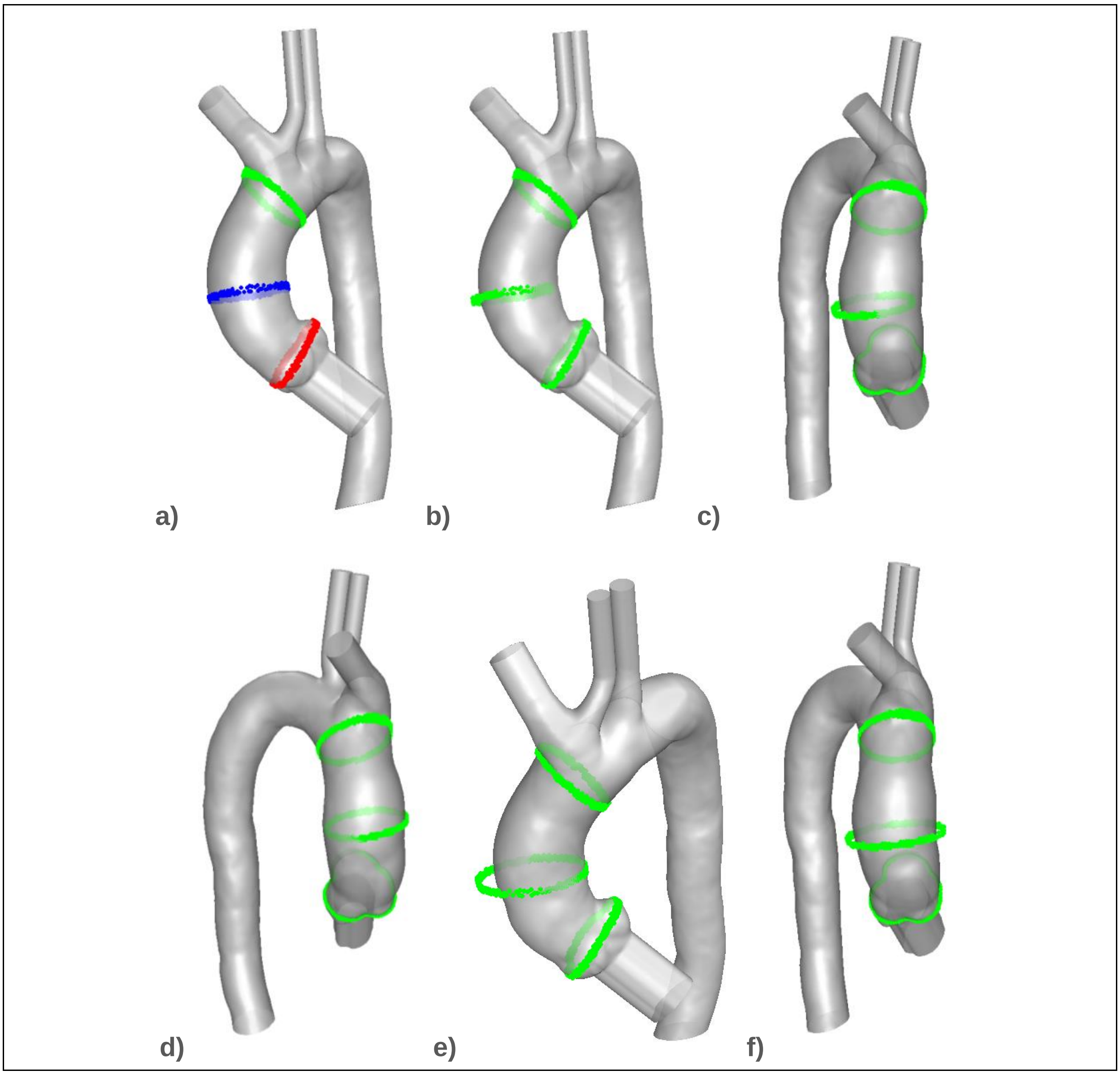

Figure 3: RBF set-up. Source points and their displacement

ROM set-up

As previously described, the ROM extraction process requires that a number of high fidelity snapshots are evaluated. Since for this problem 5 shape parameters were taken into account, and the number of snapshots must be chosen in order to catch all the important characteristics of the system, 40 snapshots were taken, selecting the Kriging method in order to seed the DP in the parameter space. The first 5 orthogonal modes were extracted with POD, obtaining a model reduced to 5 DOF. Only 5 modes were extracted since the error introduced with respect to using 10 modes is below 1%, as shown in figure 4 where the pressure results obtained using 5 modes (top row) are compared to the ones gained employing 10 modes (bottom row). This comparison was done varying the flow according to three levels of accretion of the aneurism.

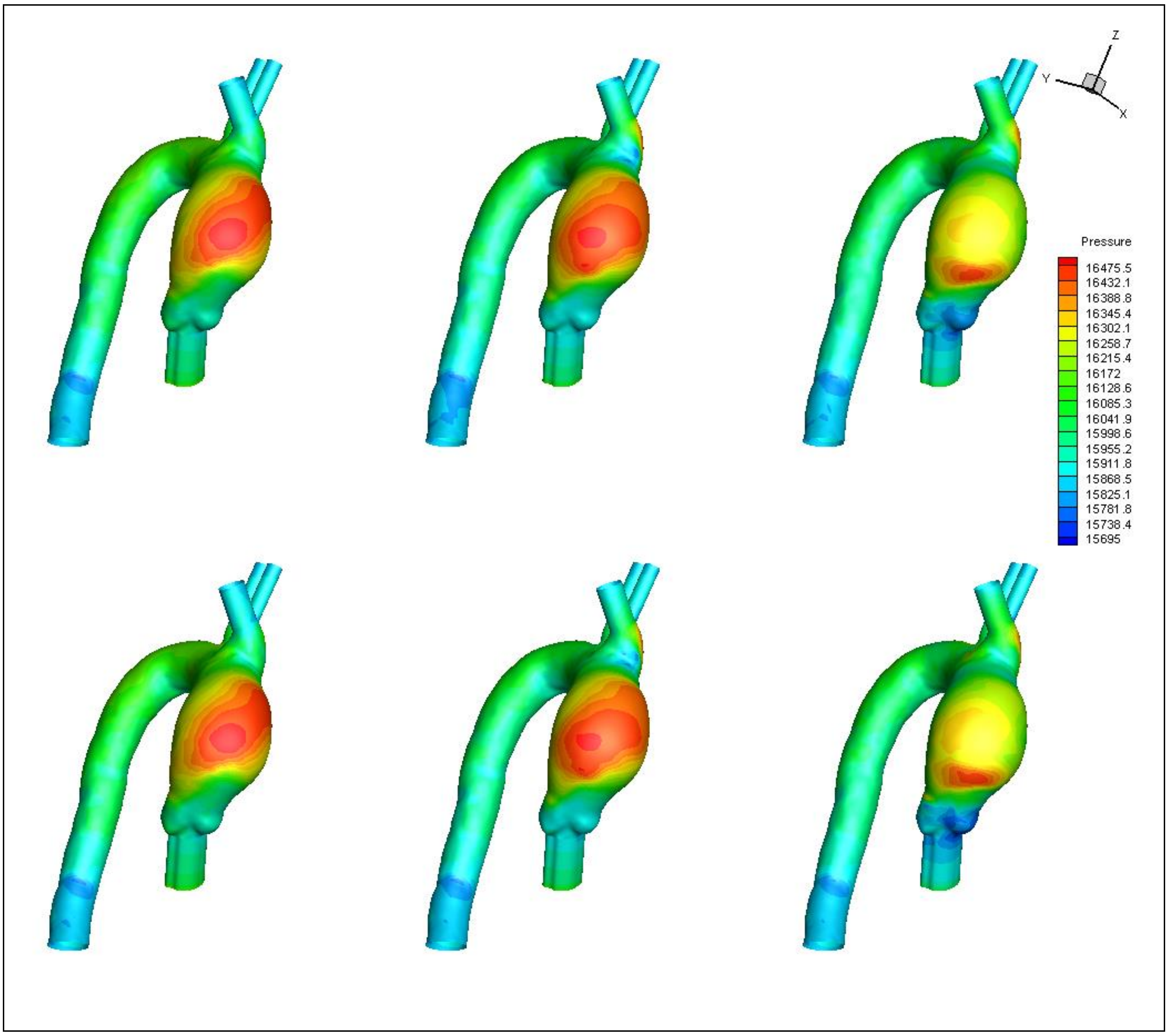

Figure 4: ROM results with 5 modes (top) and 10 modes (bottom)

Results

To assess the quality of the proposed methodology, the results obtained with the use of ROM were compared to those achieved using plain CFD evaluations. In figure 5 the pressure contours and streamlines obtained through ROM are shown for three degrees of accretion of the aneurism in the first row, while the ones calculated using a full CFD computing are shown on the last row. The maximum discrepancy between the two methodologies is in the order of 2.5%. Although this error can be further decreased by enriching the number of snapshots and employing an higher number of orthogonal modes, it sounds acceptable because each new ROM evaluation can be visualised in almost real-time while the CFD calculation requires about half an hour.

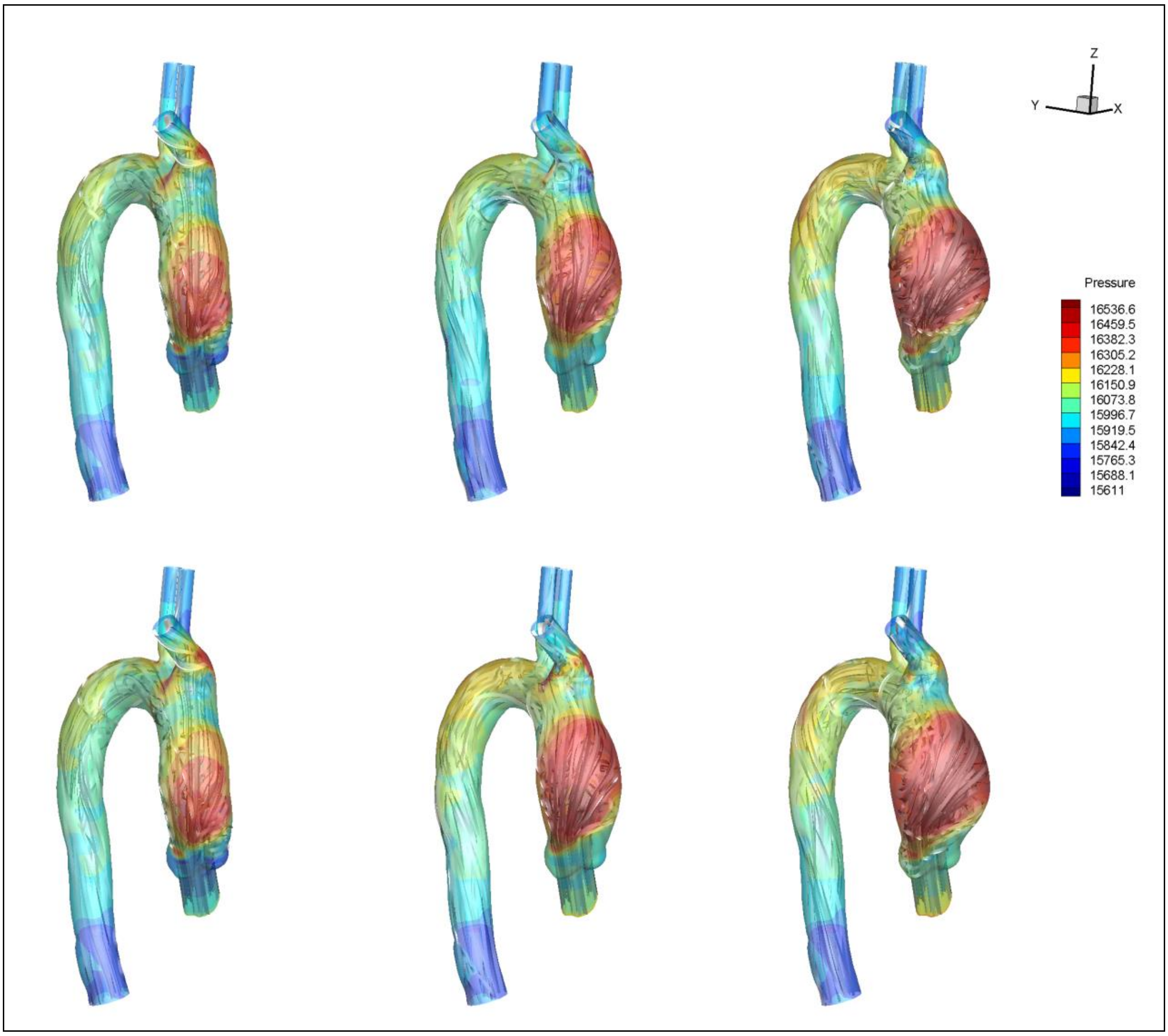

Figure 5: ROM results (top) compared to CFD (bottom)

Conclusions

The activities described in this paper deal with a critical aspect of digital twins: the need to gain computational results in real-time. Since high fidelity CFD simulations, which already proven to be useful in predicting growth and evolution of CVD pathologies, require a lot of computational efforts, a methodology to overcome this problem was proposed. ROM has proven to be very efficient in reducing computing cost for complex multi degree of freedom models (like CFD models). On the other hand, RBF mesh morphing has proven an high efficiency in generating different shapes for numerical models, thus reducing the time requested to generate a new one. The proposed methodology envisages the synergic use of ROM and RBF mesh morphing to generate, from a discrete set of shape configurations, a new shape for the CFD model with numerical results included. The proposed methodology was developed in the ANSYS® Workbench™ 19.1 environment exploiting ROM functionalities provided by this software release, and the RBF-Morph™ Fluent® add-on. The complete workflow was tested in a CFD study of an ascending thoracic aortic aneurysm. Results obtained with the proposed approach were compared to CFD evaluations, which required the full CFD solution of the new shapes of aneurism. A good agreement in term of monitored variables was finally obtained.

The successful application of the proposed methodology lead to the conclusion that it can be successfully exploited to assist the generation and fruition of digital twins in medical applications.

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