Embedded CFD Simulation for Blood Flow

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ABSTRACT

The aim of the study is the analysis of strategies and parameters to automate CFD simulations. The idea is to perform an Embedded CFD simulation for product development and verification. This work focuses on biomedical problems, in particular on vessel bifurcations with aneurysm located in the circulatory system. The research is conducted by the analysis of the pre-processing, solving and post-processing steps, in order to find a methodology that involves the reliable calculation of the CFD variables. For the pre-processing step, spatial grids study is conducted to find the element density that allows efficient calculations. The evaluations are done on a blood flow through an ideal artery bifurcation aneurysm. Subsequently the time step entity and the maximum inner iteration number are studied to calculate the independent variables. The time step is evaluated on the ideal bifurcation aneurysm with a constant inlet flow velocity, while the maximum inner iteration value is evaluated on the ideal bifurcation with a time dependent inlet flow velocity. The last study of the pre-processing is conducted on a reconstruction of real artery bifurcation aneurysm, modified with the extrusion of the inlet region, that allow the complete velocity field to develop. For each one, the original and the modified models, itõs generated an unsteady simulation with set up in agreement with previous steps. A correct post-process management study done through the pulsatile non-stationary simulation. The solution data will be used for the post-processing evaluations. So pressure and velocity evaluation layouts will be identified; Wall Shear Stress (WSS) based indices evaluation layouts will be implemented in order to enable a better evaluation of the case: Time Averaged Wall Shear Stress, Oscillatory Shear Index, Relative Residence Time. Lastly it will be considered a layout about Q-Criterion evaluation. The procedures defined during the study enable a partial automation of the CFD simulations. Acquiring an arterial bifurcation aneurysm model is possible to proceed to the automatic spatial grids generation; the numeric model is used to resolve unsteady flow, set with optimal parameters. Finally it is possible to evaluate the

calculated variables by means of appropriate diagrams generation.

Keywords: CFD, KBE, Hemodynamics.
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1 INTRODUCTION

The need to automate product design, developing and validation is increasingly more important in product developing. It is worth to underline that the integration between CAD and simulation techniques is increasingly more grounded. For this reason, experts in numerical simulation and geometrical modeling are required. Process automation is the use of procedures, rules and systems integrated into a process that automatically gives the solutions required. As a result, these systems are able to replace those activities that require the intervention of an expert of CAD/CAE systems.

Numerical simulations play an important role in the product development and they are useful as decision-making tools in many fields [18,20,29]. The numerical simulation is effective when it is usable by the designer himself and found to be an instrument of active support for the design itself. The usability of the numerical simulation is that if you can remove the classic workflow involving the presence of many specialists in the field of the CAD process, development of the numerical solvers and data analysis. To create an automatic process of product development based on numerical simulation is necessary to create awareness of management issues of the various stages of simulation, and then define the rules to help manage the process. Numerical simulations become so embedded in the product development workflow.

A possible example of the use of an automatic process with Computational Fluid Dynamics as tool for product development and diagnosis is in the field of the health. The object of interest is focused on the prognosis of aorta aneurysm disease. Many CFD approach have been investigated as an aid tool for the investigation and the prognosis concerning blood flow disease [8]. The proposed technique for the grid generation is based on a hybrid type, filling the geometry with tetrahedral and hexahedral elements. The discretization procedure is semiautomatic and it is guided by the imposition of the dimension of the cell-based edge of the grid. By this way, it is possible to obtain a very high quality grid for CFD simulation.

A definition of the steps of a process for blood flow simulation in proposed in [36] by Taylor, which shows the development of an integrated simulation using finite elements methods. The system, based entirely on KBE, shows the possibility to obtain 3D simulations having as a starting point the biomedical analysis 3D images. This demonstrates the validity of the process but do not point out the rules of the knowledge-based system. CFD analysis of a stationary flow with simplified geometric reconstruction of carotid bifurcation [5] has permitted to obtain information about the implication of Kawasaki syndrome. The critical flow regions have been investigated to understand the causes of possible formation of rupture in presence of stenosis and aneurysm. The location of the presence of the aneurysm influences the flow system reducing blood flow in the branch where the aneurysm is located.

An evaluation of the operation of endovascular embolization can be seen in the article proposed by Byun [7]. In particular, numerical simulations were performed using a Newtonian fluid model, with time dependent fluid flow modeled at the inlet of the numerical model based on an experimental investigation over patients. Through the CFD it was possible to verify the change in flow due to the insertion of coils into the aneurysm. It is shown that the influence of the fluid model, considering the blood as Newtonian or non-Newtonian one, is low and the difference in prediction of WSS and pressure was low [37]. But, considering an extended arterial system and not only the branch affected by a disease, it is possible to simulate the entirely blood flow and identify, for example, effective drug delivery methods. 3D simulations for these problems have a high degree of accuracy; however they have a high computational cost and the attendance of a CFD specialist is required. Typically, the scale of the problem is lowered from 3D model to 1D/0D models. Grinber [15] shows how using a 1D model with appropriate boundary condition, the results can be useful in clinical practice. It is not well investigated if it is possible to lower the problem from 3D to 2D, considering, as an example, the mid plane of the geometry. In reality, however, the blood vessels are not simple rigid walls but they are relatively free to move and deform. Studying the effects of fluid-structure interaction [37] proves the strong dependence of WSS and in simulation with rigid solid walls the right value of stress is overestimated. In addition, the boundary conditions of the CFD simulation affect the prediction of the variable of interest. In fact, considering an average velocity of blood flow or a pulsatile time dependent blood flow, the difference for the prediction of WSS and pressure are very important.

An important variable for the evaluation of an aneurysmal problem is the WSS, which can change the morphology and orientation of the endothelial reticule [23,24], tissue that constitutes the wall of blood vessels. Tissues subjected to laminar flow with high levels of WSS tend to stretch and align in the same direction of flow, while flows in areas with irregular grids has distorted the fabric without a clear orientation and lack of intercellular junctions. The hemodynamic forces play an important role in the development of diseases of the blood vessels. It is been shown that low values of average cut and marked fluctuations in the flow direction, can be critical factors for the emergence of atherosclerotic plaques, i.e. plaques of lipid material that can clog blood vessels and lead to serious diseases.

To take into account these factors, have been implemented indices based on the value of the indices of WSS. The Time Averaged Wall Shear Stress index (TAWSS) [23,24] represents an average temporal variation of WSS; the Oscillatory Shear Index (OSI) is used to identify areas subject to high fluctuations of WSS during the cardiac cycle. Low OSI values occur where the flow perturbations are minimal and high OSI values (maximum 0.5) while highlight areas where WSS deflects instantaneously from the direction of the main flow, causing disruption of the alignment of endothelial tissue. Q-criterion measures the vorticity of the blood flow during the motion and the criterion is used to see possible region of vorticity fluctuations that have an effect on WSS. When Q is positive means that the area where it is detected is dominated by vortex [16,19], and where Q is negative means that the flow is distributed according to its gradient. In CFD simulations the following points must be stated

- Geometry of the model;
- Grid topology and discretization strategy;
- Solver setup and visualization.

Blood vessel geometry reconstruction by biomedical analysis is the first step in an embedded process in vascular simulation. This issue is not discussed in this work, since the focus is on the estimation of the rules for numerical grid generation, solver setup and visualization for diagnosis.

Moreover, this piece of work deals with the problem concerning the choice between geometric and discretization calculation of 2D or 3D models [2,4,13,15,25]. A 3D geometry and its related tri-dimensional calculation grid, take longer calculation times than a 2D grid. Obviously, the results obtained are different. The issue is to measure such gap and to find out how to adopt reduced geometric models and computational grids. It has also been investigated the problem of the discretization [21,26,33] and the effect of the geometrical variations, which is vessel geometry-sensitive (diameter, etc.) [9,17].

This study aims at finding out a possible approach to make work such tools in the so-called “embedded simulation”, here “Embedded CFD”. The latter is an automatic simulation, which is integrated to the medical investigation system. In this way the abovementioned problems may be solved. Although the technologies have reached a good level of improvement, such approach has not been fully developed as well as it seems difficult to be implemented. Embedded CFD simulations for blood flow are grounded on these rules:

- CAD reconstruction from medical images;
- Grids topology and cells size based on the geometry dimension;
- Numerical solver settings (time step and number of internal iteration) for each step;
- Visualization of the data for decision-making.

In this work we define some rules useful to understand the problem and to develop the procedure in a prototype based on ȍEmbedded CFDȎ.

In the following, we first provide a brief introduction on fundamentals to simulate blood flow, then, section 3 describes rules extraction to automate CFD analyses finalized to aneurism study and, finally, conclusions are reported.

2 NUMERICAL METHOD

The equation resolved by using CFD are derived from the fundamental laws of fluid mechanics [27,35], that are:

- Conservation of Mass;
- Conservation of Momentum;
- Conservation of Energy.

The differential form of the equation of Conservation of Mass is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{v}\right) = 0 \tag{2.1}$$

It states the mass of the control volume is preserved. If the fluid is assumed as incompressible one, the conservation of mass equation becomes $\nabla \cdot \vec{v} = 0$, and it is valid for steady and unsteady flow.

In Lagrangian reference system, the equation of the Conservation of Momentum is:

$$\frac{d\left(M \cdot \vec{v}\right)}{dt} = \sum_i F_i \tag{2.2}$$

It says that the momentum variation is due to the forces acting on the flow. The differential form of the equation is:

$$\frac{\partial \rho \vec{v}}{\partial t} + \vec{v}\left(\nabla \cdot \vec{v}\right) - \rho \vec{g} + \vec{\nabla} p - \vec{\nabla} \cdot \vec{\vec{\tau}} = 0 \tag{2.3}$$

Combining the first and the second equations into a system, we can resolve it using a numerical scheme. The following equation are called Navier-Stokes equations:

$$\begin{cases} \nabla \cdot \vec{v} = 0 \\ \dfrac{\partial \rho \vec{v}}{\partial t} + \vec{v}\left(\nabla \cdot \vec{v}\right) - \rho \vec{g} + \vec{\nabla} p - \vec{\nabla} \cdot \vec{\vec{\tau}} = 0 \end{cases} \tag{2.4}$$

2.1 Hemodynamic Index

The method for the calculation of index is reported in [23,24]. The calculation of the TAWSS index shall be carried out with the formula based on the integral in time of WSS over the simulation period, for each point to the wall: this integration can be carried through the most common rules of numerical integration, as the composite trapezoidal rule or the rule of the midpoint the composite. For our calculation has been chosen to adopt the rule of the midpoint, as it is easier to implement and provides less error than the trapezoidal rule [30]. Integration is then performed point to point according with:

$$TAWSS = \frac{1}{T}\int_0^T \left|WSS\left(s,t\right)\right| \cdot dt \tag{2.5}$$

The OSI index is defined as:

$$OSI = 0.5 \cdot \left[1 - \left(\frac{\left|\int_0^T WSS\left(s,t\right) \cdot dt\right|}{\int_0^T \left|WSS\left(s,t\right)\right| \cdot dt}\right)\right] \tag{2.6}$$

Q-criterion, according with [7], is a scalar quantity defined by:

$$Q = \frac{1}{2}\left[\left\|\Omega\right\|^2 - \left\|S\right\|^2\right] \tag{2.7}$$

where S is the strain-rate tensor and Ω is the vorticity tensor.

3 RULES EXTRACTION AND DISCUSSION

To study the rules related to CFD simulation, it was decided to use a simpler geometry as a benchmark able to explain the object of interest [5]. In fact, this model makes simpler the problem for the study of the automatic procedure. Figure 2 shows the CAD model of branch of an artery with an aneurysm located on the LCA branch. The model allows representing the main branch coronary (LAC), bifurcations (LAD, LCX) and the presence of a disease, in particular, an aneurysm.
The branch are modeled as circular pipe and LAC, LAD, LCX section diameter is 6*mm*; the aneurysm is modeled as a sphere with diameter of 20*mm*. An angle of 60° is formed between LAD and LC branches. Rigid and impermeable walls are the boundary conditions for the vessel walls.
An automatic discretization algorithm was used to generate the numerical grids. The procedure is based on the knowledge of the geometrical dimensions. In particular, it allowed the automation of the procedure of mesh generation with refinements zones congruent with the vessel geometry. All the generated grids are hybrid grids, with a prismatic layer near vessel walls and tetrahedral or hexahedral elements inside the vessel.

The fluid is considered as human blood as Newtonian fluid. For the preliminary studies, the fluid velocity is considered constant. The numerical scheme for coupling velocity and pressure is a segregated type. Fluid properties are shown in Table 1.

In according with [5], the investigation for CFD rules is performed using the average velocity inside the vessel and the diastolic velocity (Table 2).

Density [kg/m³]	*1050*

Viscosity [kg/m-s]	*0.0035*

Tab. 1: Blood properties as Newtonian fluid.

Velocity [m/s]	*0.14*	*0.25*
Reynolds	*250*	*450*

Tab. 2: Inlet velocity conditions tested and related Reynolds numbers.

A steady state simulation was performed for each tested velocity. The boundary conditions are show in Figure. Red surface is a boundary condition of velocity inlet with flat constant velocity; Blue surfaces are modeled as pressure outlet and the vessel walls are modeled with no-slip condition.

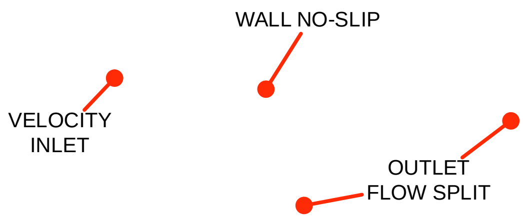

Fig. 1: CFD model boundary conditions.

For the preliminary analysis, the velocity profile and the maximum velocity inside the vessel are used as scalar quantities of interest. The probe line for velocity monitoring is show in Figure 2.

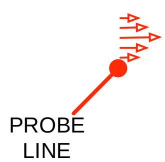

Fig. 2: Line probe position.

3.1 Grid Topology V&V

The Verification and Validation procedure proposed by [38] was performed on the 3D benchmark geometry explained before. This geometry has many simplification compared to one obtained from TAC analysis and unfortunately we don't have any experimental data, so the procedure is limited to the verification phase of the grid. Three grids with Non-Conformal Hexahedral elements and four grids with Polyhedral elements were tested. In table 3-4 is reported the grid sizes for each type of grids tested. Figure 3 show a sample of mesh generation with hexahedral elements.

Non-Conformal Hexa	*CV*
Fine	1.767.844
Medium	981.894
Coarse	371.920

Tab. 3: Grid size for non-conformal hexahedral grids.

Polyhedral	*CV*
Fine 1	4.254.911
Fine 2	1.602.206
Medium	482.203
Coarse	170.503

Tab. 4: Grid size for polyhedral grids.

Fig. 3: Non-conformal Hexahedral grid.

In Figures 4, the maximum velocity inside the vessel is reported as a non-dimensional number, obtained dividing that by the scalar quantity obtained from the simulation with base grid.

Using the guidelines in [34], we perform the calculation of the uncertainty and the orders p of convergence of the grid. Also, uncertainty bars with 95% of confidence are showed

The verification procedure was performed at different velocities, resulting in Re = 250 and Re = 450. As a result, the V&V procedure indicate the best grid topology for implement an automatic process of discretization; it is possible using non-conformal hexahedral grids with normalized cell size by inlet diameter of 0.425 (Table 5).

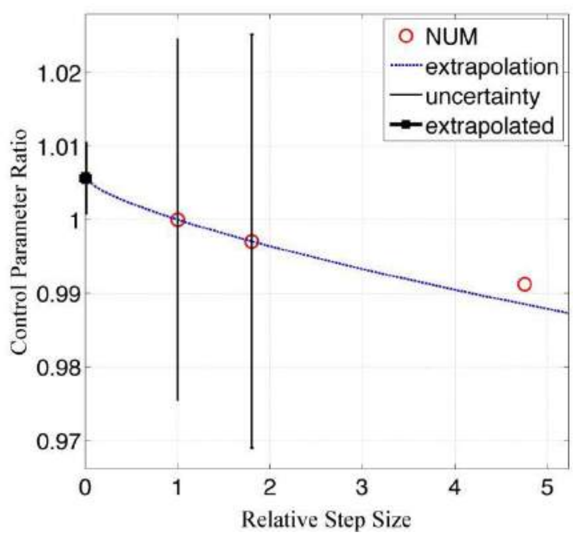

Fig. 4: Re=250; non-conformal Hexahedral grids maximum velocity variations vs. spatial resolution.

Parameter	*Rule*
Grid Type	non-conformal Hexahedral
Cell size dx/D	0.425
Prism layer	8 elements

Tab. 5: Rules for hexahedral meshing.

3.2 Solver: Time Step e Iteration

The systematic study of the computational grid has allowed us to derive the rules of spatial discretization based on a geometrical parameter, the diameter of inlet branch. Now it is necessary to determine which are the rules for the time discretization, because blood flow is not constant over time but is subject to a periodic cycle.

To study the influence of the time step, we have generated a family of non-stationary simulations, based on rules derived from the spatial discretization seconds earlier study, which only differ in the value of the control parameter time of the numerical solver. As for the study of the grid, the ratio of the refinements of time step is constant.

The cardiac cycle is simulated under the assumption of Womersley [36], defining the velocity versus time according to the following law:

$$V_{in} = V_{med}\left(1 + \sin(2\pi \frac{t}{T})\right) \tag{3.1}$$

with Vmed=0.14m/s, T=0.8s.

The parameter of comparison is the maximum velocity inside the vessel. By comparing the numerical errors due to time discretization, Figure 5, we note that the performance reaches a minimum at $e45$, then change slope and increase the value of the error. This means that you have reached the limit of refinement of the variable time and a subsequent refinement gives a numerical oscillation results.

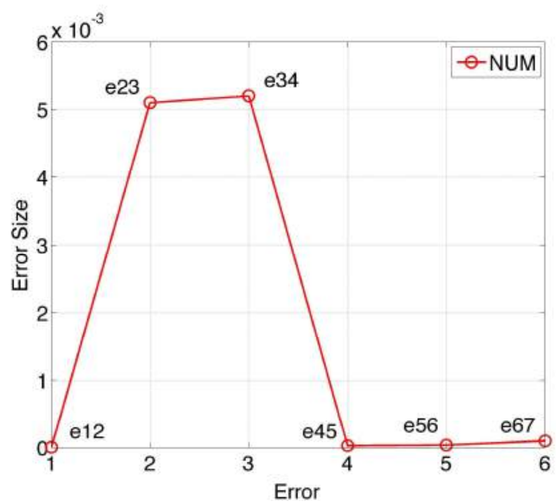

Fig. 5: Time Step error.

With V&V procedure [38], we found that the optimal time step for this type of simulation with laminar blood flow is *dt=0.00125s*.

As mentioned previously, the error due to a numerical simulation consists of three components: rounding errors, discretization errors and iteration error [34]. Derived the rules of discretization (in time and space) is necessary to establish the rules for the numerical solver. The control parameter in this series of simulations is the number of iterations for each time step; 5, 10, 20 iterations per time step is the setup of control parameter.

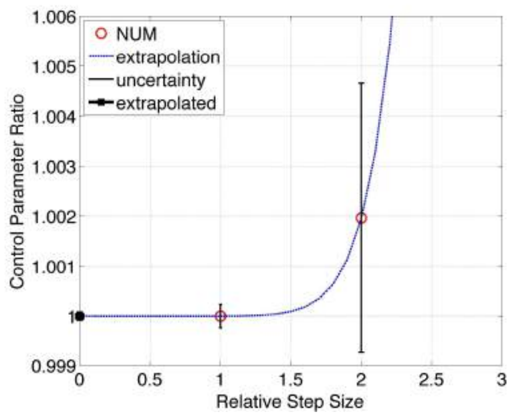

Fig. 6: Maximum velocity variation vs. inner iteration resolution.

The maximum velocity versus time is monitored and used for the derivation of the rule in iteration procedure. In Figure 6 shows the graph of the convergence for the number of iterations. It can be concluded that 20 iterations for each time step guarantees the lowest error range of uncertainty, combined with a high order of convergence.

3.3 Boundary Conditions

In order to use the rules of spatial and temporal discretization obtained through systematic study, it was decided to set up the CFD analysis using a reconstruction of a real coronary artery bifurcation, Figure 7.

Fig. 7: CAD reconstruction of real bifurcation aneurysm.

As the geometric reconstruction is faithful, the numerical simulation leads to simplifications that can lead to discrepancies of similarity between the virtual model and the real case, in which the bifurcation is not truncated at both ends but is connected to the circulatory system. For this reason it was decided to assess any changes to the actual geometry, to bring the numerical simulation to the real problem: a first amendment concerns the extrusion of the inlet region, in order to give the model a developed velocity profile. The first step in changing the geometry is to understand what length of a circular duct has a flow with fully developed velocity profile in the axial direction. The reference geometry for this systematic study is a circular duct of diameter D=0.2m e length L=8m. The tests are set with input conditions involving stationary regimes characterized by Re=252 and Re=450. The value of the maximum axial velocity is monitored in different sections.

The purpose is to check the section in which the maximum speed does not vary more according to the axial dimension, considering the flow so fully developed. This makes it possible to obtain the ratio of length to diameter, which guarantees that condition.

From the results we see that a ratio L/D=20 is sufficient to extrude the edges of the virtual model of blood vessels in laminar regime. A greater length of extrusion would increase only the number of grid elements, increasing the computational cost of simulation.

This rule of geometric modification is applied to the geometry reconstruction of the real bifurcation. The geometry has an inlet diameter of D=1.4cm, so the length of extrusion is equal to $L \cdot D = 28cm$. Two lines probe inside the aneurysm are generated to monitor the velocity magnitude for each geometry. The extrusion of the inlet region of the 3D model determines the differences in the velocity gradients, pressure and WSS. Geometry without inlet extrusion, presents an under-estimation of the flow structure in the inlet branch, leading into the aneurysmal sac because the blood flow is not fully developed (Figure 8-9).

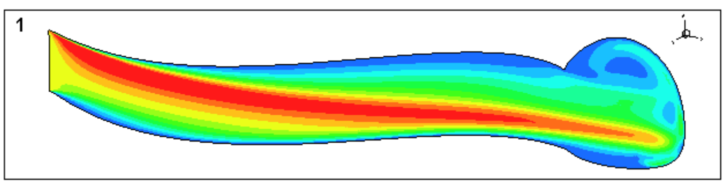

Fig. 8: Velocity magnitude plotted on mid-plane of inlet branch for real geometry.

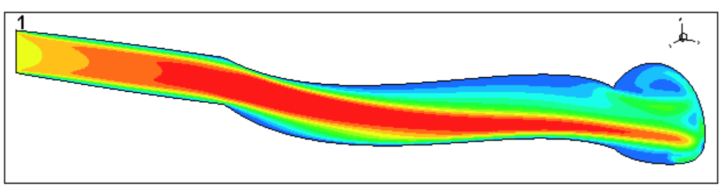

Fig. 9: Velocity magnitude plotted on mid-plane of inlet branch for modified geometry.

3.4 Visualization

For the visualization of the numerical solution, is very simple to plot scalars gradient over surfaces of the vessel or inside the same vessel. The Embedded CFD simulation should produce a result that can indicate possible diseases. The rules for this step are to implement some hemodynamic indices useful for this type of problems.

A Python script executes the time integration of the WSS and the calculation of the indices. Also, the script assesses a graphical layout for numerical solution representation. Figures 10-12 are a good example of layout representation useful for clinical diagnosis.

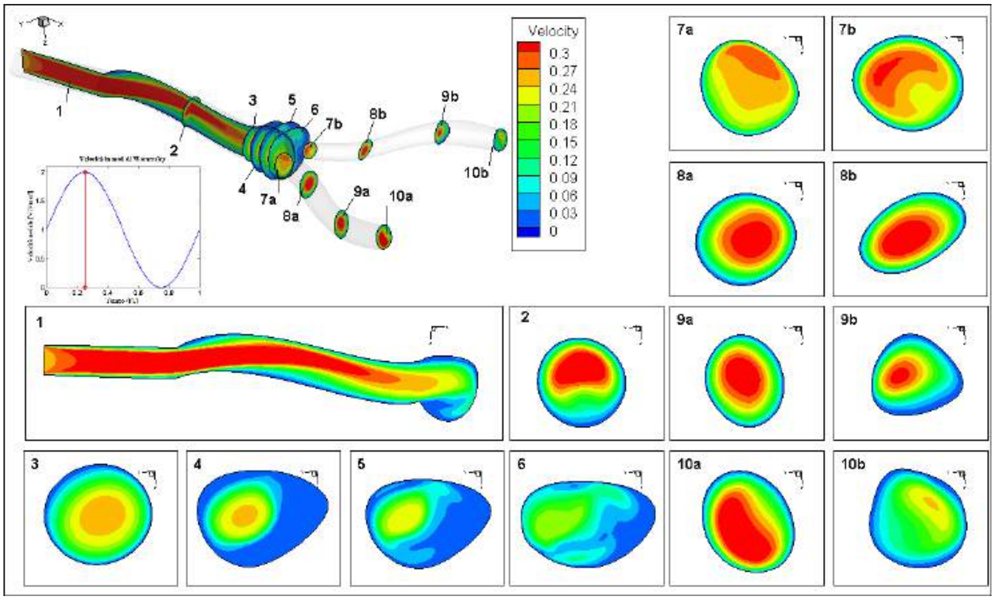

Fig.10: Layout for maximum velocity.

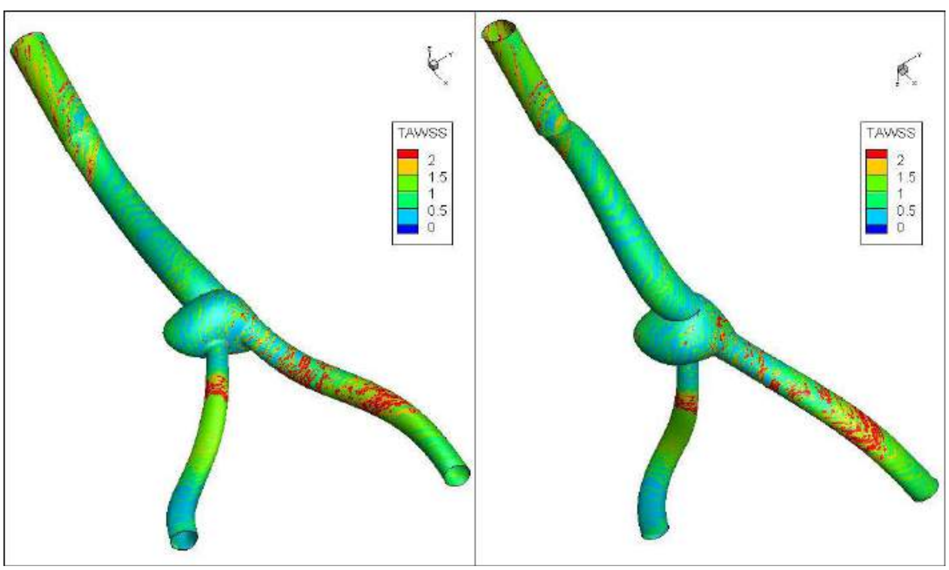

Fig. 10: Layout for TWASS index.

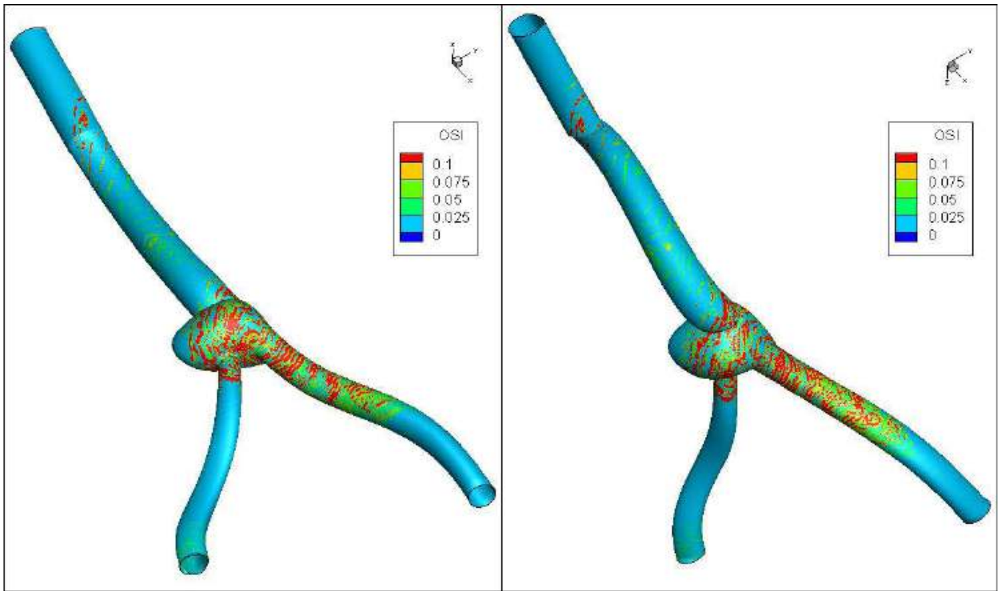

Fig. 11: Layout for OSI index.

4 CONCLUSIONS

The study has allowed the construction of the rules used in numerical simulations of blood flow in coronaric bifurcations affected by the presence of aneurysm. These rules are useful to develop an integrated CFD simulation, or "Embedded CFD", automatic process, which contains the rules and procedures for grid generation, the solver settings and the generation of parametric images useful to the scientific visualization. Through this system, the CFD tool can be made accessible, for example, to the doctors, that they can extract useful information such as diagnosis and prevention without intervention of a numerical fluid dynamics expert

The investigation has focused primarily on issues related to the generation of the grid for CFD analysis. The numbers drawn from the rules have allowed the estimation of the best grid topology to be used for this type of problems. The cell size is a key parameter for the quality of the numerical results. The study of the grid was allowed to derive a rule related to the geometrical size of the vessel and so to define the optimal size of the cell.

We also investigated the influence of boundary conditions, evaluating the effects of a change in the geometry. The input and output sections have been extended to ensure that within the aneurysm, blood flow arrives already fully developed. The rule for changing the geometry was obtained using steady laminar flow simulations in pipes, in which section of it happening the velocity profile is fully developed.

Subsequently, the rules were designed to make the numerical solver setting. The main rules are related to the time step size and the relative number of internal iterations per cycle. We found an optimal time step and optimal number of internal iteration per time step.

Finally, implementing the hemodynamic indices and obtaining layouts useful in the diagnosis of the patient carried out the procedure for post-processing and scientific visualization.

The results obtained are assumed to be able to get an automatic process for a fluid dynamics simulation, which has as its basic input medical image acquisition and as a result a layout with interest scalar quantities, such as velocity distributions, WSS and hemodynamic indices, useful for the medic. These parameters can be important for the selection of the best therapy to be submitted to the patient.

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