



TRABAJO DE FINAL DE GRADO

Bachelor's degree in Mechanical Engineering

**PATIENT-SPECIFIC NUMERICAL SIMULATION OF BLOOD
FLOW IN PULMONARY ARTERIES WITH IN-VIVO
VALIDATION**



Memoria y Anexos

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Abstract

Understanding and detailed visualization of fluid dynamics in the cardiovascular system has become a very active area of research in biomedicine. It is known that blood flow plays a key role in the proper functioning of the cardiovascular system and in the progression of the related pathologies. For this reason, computational fluid dynamics simulations have become increasingly important in the field of Cardiovascular Medicine. Given the limitation of current imaging methods, computational fluid dynamics has become a powerful tool for producing detailed, patient-specific information.

In this final degree thesis, patient-specific data, obtained by magnetic resonance imaging, have been used to create a three-dimensional model, which has been used to perform a computational simulation of blood flow into the pulmonary artery, using open source software SimVascular.

The principal obtained results, such as the volumetric flow during the cardiac cycle or the velocity distribution, have been analyzed and compared (graphically and numerically) with the in vivo data of the patient, observing the correlation between the two, results have been validated.

Resum

La comprensió i visualització detallada de la dinàmica de fluids al sistema cardiovascular és una àrea de recerca molt activa en biomedicina. Se sap que el flux sanguini juga un paper clau en el funcionament correcte del sistema cardiovascular i en la progressió de les patologies que l'afecten, per aquesta raó, la dinàmica de fluids computacional i les seves simulacions han anat cobrant importància en el camp de la Medicina Cardiovascular . Atesa la limitació dels mètodes d'imatge actuals, la dinàmica de fluids computacional ha esdevingut una eina poderosa per produir informació detallada i específica de cada pacient.

En aquest treball final de grau, les dades específiques d'un pacient, obtingudes mitjançant una ressonància magnètica, han estat utilitzades per crear un model tridimensional, que s'ha utilitzat per dur a terme una simulació computacional del flux sanguini a l'artèria pulmonar, mitjançant l'ús del programari lliure SimVascular.

Els principals resultats obtinguts, com el cabal volumètric durant el cicle cardíac o la distribució de velocitats, han estat analitzats i comparats (gràfica i numèricament) amb les dades in vivo del pacient, de manera que, observant la correlació entre tots dos, s'han pogut validar els resultats.

Resumen

La comprensión y visualización detallada de la dinámica de fluidos en el sistema cardiovascular es un área de investigación muy activa en biomedicina. Se sabe que el flujo sanguíneo juega un papel clave en el correcto funcionamiento del sistema cardiovascular y en la progresión de las patologías que le afectan, por esta razón, las simulaciones computacionales de dinámica de fluidos han ido cobrando importancia en el campo de la Medicina Cardiovascular. Dada la limitación de los métodos de imagen actuales, la dinámica de fluidos computacional se ha convertido en una herramienta poderosa para producir información detallada y específica de cada paciente en particular.

En este trabajo final de grado, los datos específicos de un paciente, obtenidos mediante una resonancia magnética, han sido utilizados para crear un modelo tridimensional, que se han utilizado para llevar a cabo una simulación computacional del flujo sanguíneo en la arteria pulmonar, mediante el uso del software libre SimVascular.

Los principales resultados obtenidos, como el caudal volumétrico durante el ciclo cardiaco o la distribución de velocidades, han sido analizados y comparados (gráfica y numéricamente) con los datos in vivo del paciente, de forma que, observando la correlación entre ambos, se han podido validar los resultados.

Acknowledgements

To Francesco Capuano, project director, who has guided me throughout the development of the work and has resolved all the doubts that have arisen. Thanks to him, I have been able to acquire new knowledge that will surely be useful in the future. I appreciate all the time he has spent on me and my thesis.

I would also thank my family and friends for all the support they have shown me throughout the course of the degree.

Glossary

PC - Pulmonary circulation

MPA - Main pulmonary artery

LPA - Left pulmonary artery

RPA - Right pulmonary artery

CFD - Computational fluid dynamics

MRI - Magnetic resonance imaging

BCs - Boundary conditions

In vivo - Medical procedures, tests, and experiments that researchers perform outside of a living organism

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1. Introduction

The detailed visualization and understanding of blood flow dynamics in the cardiovascular system is a very active research area in biomedicine. Blood flow is known to play a key role in maintaining normal function and in modulating the progression of pathologies, for this reason, numerical simulations of computational fluid dynamics have been becoming more important in the field of Cardiovascular Medicine.

Given the limitation of current imaging modalities, patient-specific computational fluid dynamics (CFD) has emerged as a powerful tool to produce detailed flow information. In this approach, the vessel geometry is extracted from clinical data of the patient (e.g. magnetic resonance) and used to build a three-dimensional computational model wherein the Navier-Stokes equations are numerically solved with proper initial and boundary conditions.

In this project, 3D time-resolved magnetic resonance imaging ("4D flow") is combined with CFD to study the detailed three-dimensional features of blood flow.

1.1. Goals of the project

The principal objective of this work is to obtain a more detailed understanding of the behaviour of blood flow in a patient-specific pulmonary artery through numerical simulations with the finite element program SimVascular.

Another of the main objectives of this project is to validate the used CFD software.

2. Cardiovascular system

The cardiovascular system is an organs system formed by heart, vessels and blood which his function is to supply the human body with oxygen and nutrients. The cardiovascular system has two divisions, a systemic circuit and a pulmonary circuit (to which the pulmonary artery belongs).

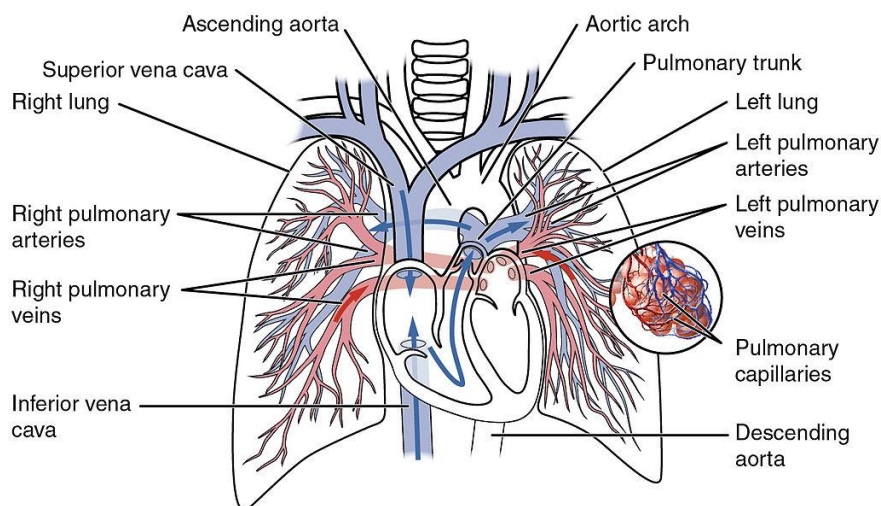


Figure 2.1: Schematic of the pulmonary circuit.

The pulmonary circuit is the responsible to oxygenate the blood; the circuit begins with deoxygenated blood returned from the body to the right atrium of the heart, where it is pumped out from the right ventricle to the lungs. In the lungs, the blood is provided with oxygen and returned to the left atrium to complete the circuit. In normal conditions, it is a low-pressure (15 mmHg pressure difference), low-resistance, high-flow system.

2.1. Pulmonary artery

The main pulmonary artery, also called the pulmonary trunk, is a relatively short and wide artery, having a length of only about 5cm. Located at the exit of the right ventricle that collects the poor-oxygen blood from the ventricle and carries it into the lungs, where oxygen enters the bloodstream.

It is divided in right and left branches, which sends blood to the right and left lungs, respectively. His shape is very similar to a capital letter "T".

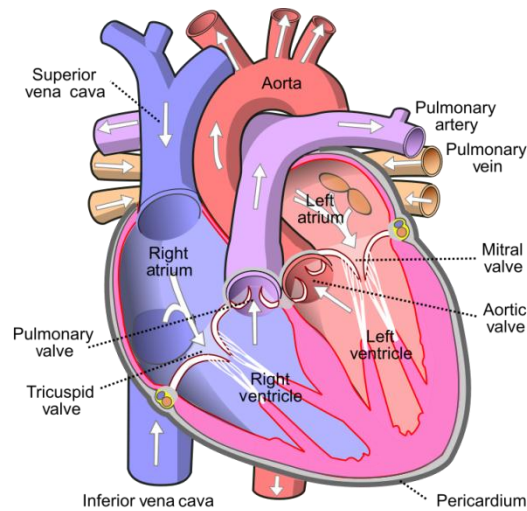


Figure 2.2: Frontal view of opened heart. Arrows indicate normal flow (Pulmonary artery labelled at upper right).

The right pulmonary artery runs underneath the aortic arch and passes behind the superior vena cava to the right lung.

The left pulmonary artery is shorter than its right counterpart and arches over the left main bronchus before reaching the left lung.

2.2. Blood as a fluid

Blood can be defined as a real, non-Newtonian fluid, with pulsatile blood flow in large arteries and susceptible to developing turbulence at bifurcations.

Instead, in our simulation, blood will be considered a Newtonian fluid. Assuming the Fahreus-Lindqvist effect, the decrease of viscosity in small diameter pipes is not present in large-caliber vessels [2].

In general, blood flow is considered laminar and follows the Poiseuille law. The flow resistance reaches their maximum level in the vicinity of the wall, and its minimum value is located into the geometrical centre of the blood vessel.

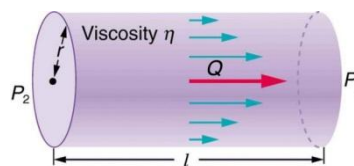


Figure 2.3: Poiseuille laminar flow representation

3. Navier-Stokes equations

Navier-Stokes equations are a system of partial differential equations that describes the motion of viscous fluid substances, mathematically, express conservation of momentum, mass and energy for Newtonian fluids.

$$\text{Mass: } \frac{\partial}{\partial t} + (\vec{v} \cdot \vec{\nabla})\rho + \rho \vec{\nabla} \cdot \vec{v}$$

$$\text{Momentum: } \rho \frac{\partial \vec{v}}{\partial t} + \rho (\vec{v} \cdot \vec{\nabla})\vec{v} = -\vec{\nabla}p + \mu \Delta \vec{v} + \rho \vec{f}_e$$

$$\text{Energy: } \frac{\partial \rho e}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v} h) = (\vec{v} \cdot \vec{\nabla})p + (k \vec{\nabla} T) + \varepsilon_v + q_H$$

Where:

\vec{v} : velocity vector (u,v,w)	$\vec{\nabla}$: gradient of divergence
ρ : density	\vec{f}_e : external force vector
μ : coefficient of dynamic viscosity	ε_v : turbulence dissipation rate
q_H : heat source	

Figure 3.1: Navier-Stokes equations

In this project, blood flow is calculated by the incompressible Navier-Stokes equations, as we consider blood a Newtonian fluid (Chapter 2.2). Adopting that thesis simplifies considerably the equations, because the specific mass may be considered as constant. This simplification, leads to a decoupling of the energy equation from the other conservation laws if the flow remains isothermal. Reducing the conservation equations to:

$$\text{Mass: } \vec{v} \cdot \vec{\nabla} = 0$$

$$\text{Momentum: } \rho \left(\frac{\partial \vec{v}}{\partial t} + \rho (\vec{v} \cdot \vec{\nabla})\vec{v} \right) = -\vec{\nabla}p + \mu \Delta \vec{v}$$

Figure 3.2: Navier-stokes equations for incompressible flows

Numerical methods are used to approximate the equations, obtaining solutions for velocity and pressure at a defined number of points. The resolution of millions of differential equations for each time-step with computational fluid dynamics (CFD) is required, defining a domain of interest formed by surfaces and volumes restricted by boundary conditions, in order to obtain a valid solution.

4. Software used in the project

4.1. SimVascular

Simvascular is software package originally developed by Stanford University to provide a complete pipeline from medical image data to patient specific blood flow simulation and analysis. Is composed by:

- **Simvascular:** Interactive image-based modelling pipeline application.
- **svPre:** is the preprocessor for svSolver. The input data files to svPre contain a complete description of the discrete model: nodal coordinates, element connectivity, element adjacency information and connectivity of boundary nodes and elements. The svPre program can be called either from the command line (in terminal) or the Simulation tool (in GUI). The input data files for svPre are created from the mesh.
- **svSolver:** Computational fluid dynamics solver (CFD). Evolved from the academic finite element code PHASTA (Parallel, Hierarchical, Adaptive, Stabilized, Transient Analysis)[5], this code is inspired by the Stabilized Finite Element theory **Error! No s'ha trobat l'origen de la referència..**
- **svpost:** Postprocessor for svSolver, transform svSolver solution files to .vtu files

4.2. Paraview

ParaView is an open-source, multi-platform data analysis and visualization application. ParaView users can quickly build visualizations to analyse their data using qualitative and quantitative techniques. The data exploration can be done interactively in 3D or programmatically using ParaView's batch processing capabilities.

ParaView was developed to analyse extremely large datasets using distributed memory computing resources. It can be run on supercomputers to analyse datasets of petascale size as well as on laptops for smaller data, has become an integral tool in many national laboratories, universities and industry.

Will be used to visualize and extract Flow-rates from 4-D image data and the simulation solutions.

4.3. Matlab

Matlab is a programming language and interactive environment for numerical computation, visualization and programming. It has numerous built-in commands that help to do mathematical methods, generating plots or managing data sets.

In this project will help us to read patient-specific in vivo data, in order to visualize it in Paraview and calculating the pulsatile inflow in the simulation.

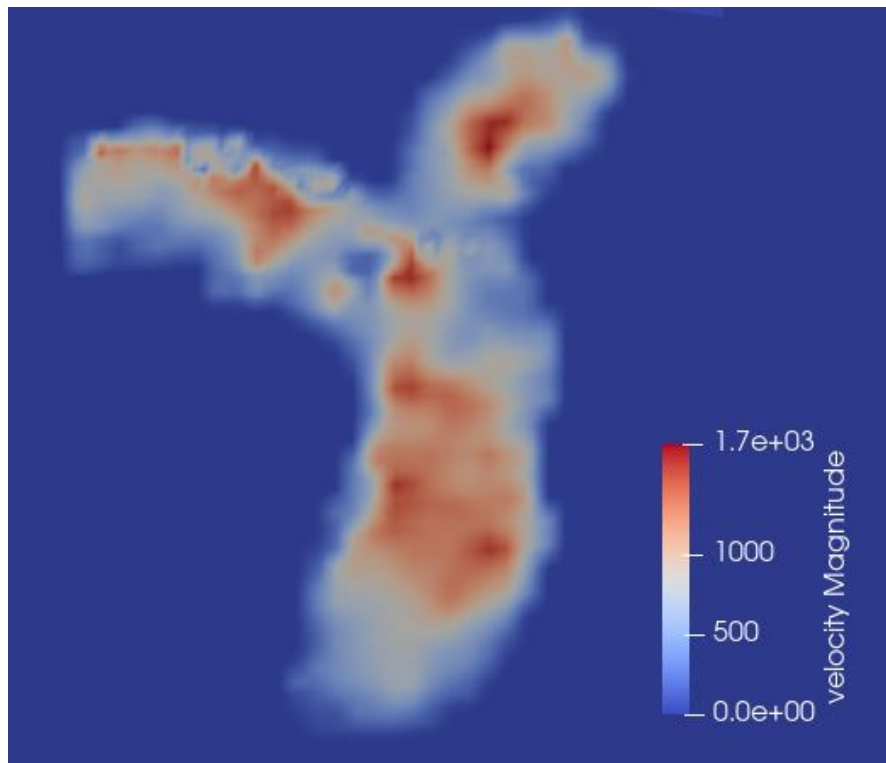


Figure 4.1: Paraview view of in-vivo velocity processed with Matlab.

5. Materials and Methods

5.1. Subject of the study

The analysed pulmonary artery is from a healthy male patient, the MRI used to get the geometry and the in-vivo velocity distribution of this project has been provided by Hospital Vall d'Hebron from Barcelona, Spain¹.

5.2. Patient-specific data - 4D Flow

4D Flow is a type of phase-contrast MRI that, as a result, gives blood velocity data in three directions, in a 3 dimensional space, and through all the cardiac cycle.

With 4-D Flow images, global and regional dynamics of blood flow can be analysed through different hemodynamic measurements (velocity, average flow, ...). This image method can also be used to analyse the temporal evolution of complex flow representations (flow lines, 3D velocity graphs and vectors, ...)which describes the trajectory of the blood, over time, in the cardiovascular system.

Those mentioned characteristics, allows that technique to have many potential clinical applications, and it provides information of the function and status of the specific cardiovascular system of patients.

Patient specific information has been used in this project for the construction of the CFD model, and also, for the configuration of some of the boundary conditions who determine the results of the simulations.

From 4-D flow image, we get the inlet and outlets velocity distribution during all the cardiac cycle (51 time-steps). Integrating those velocities, blood flowrates are obtained.

¹ Andrea Guala and Lydia Dux-Santoy (Vall d'Hebron Research Institute - VHIR) are gratefully acknowledged for providing the data used in this project.

All that data will be used to set up the next boundary conditions:

- Inlet velocity
- RPA/LPA flow resistance

5.3. CFD model

5.3.1. Geometry

Using the open-source software SimVascular, patient specific PA 3D file was imported, and using the SV “Model” section, possible holes in the surface have been filled, and the external surface has been smoothed. After that inlet, outlets and artery walls have been assigned in the model.

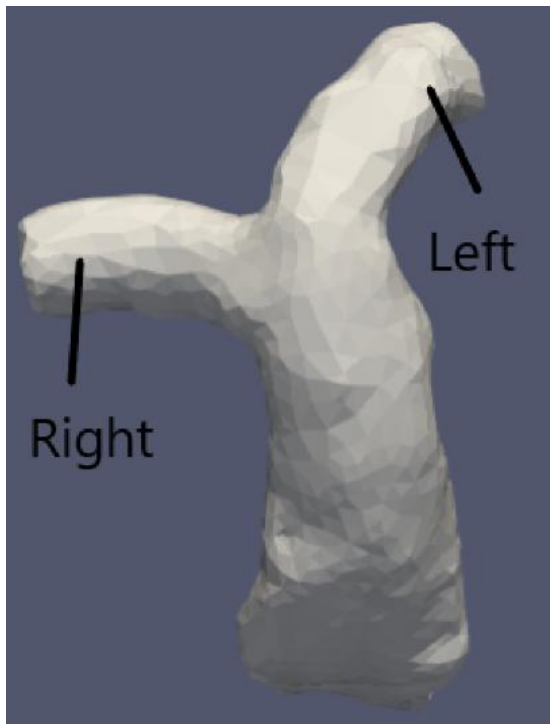


Figure 5.1: Patient-specific pulmonary artery geometry

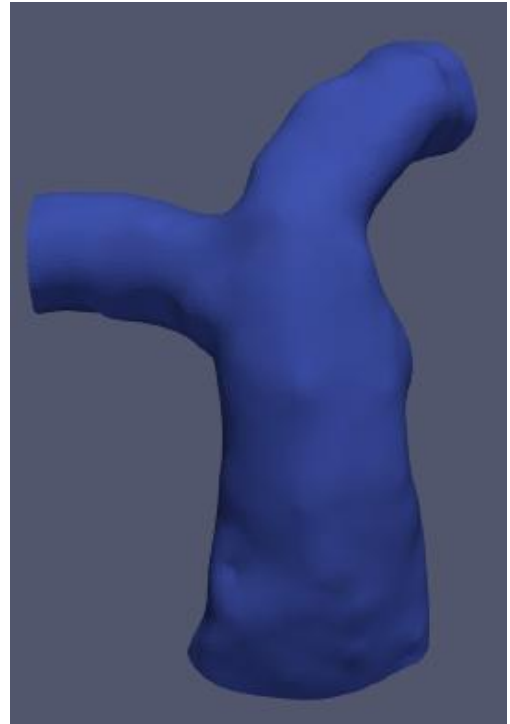


Figure 5.2: CFD pulmonary artery geometry

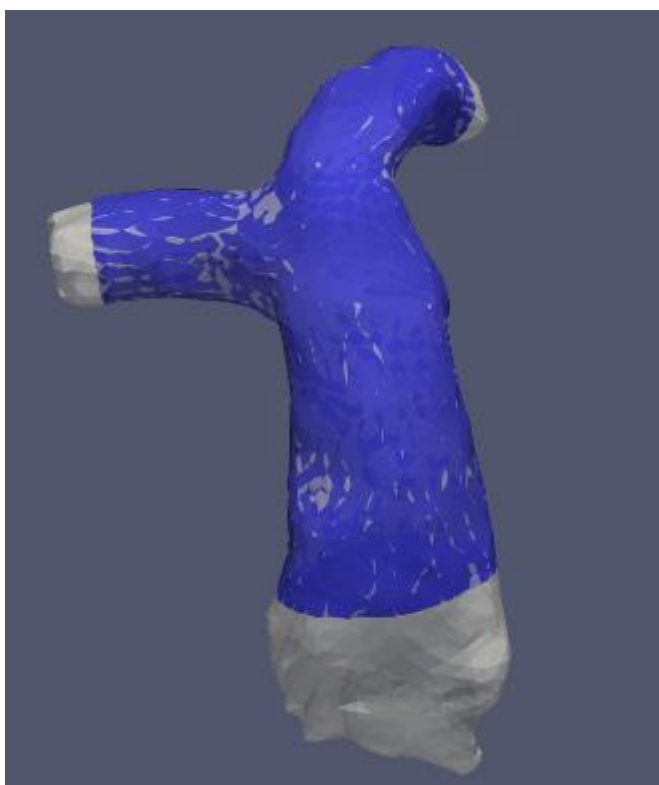


Figure 5.3: Comparison CFD – in vivo geometries

Finally, inlet, outlets and the wall of the PA model are defined in order to generate the mesh.

5.3.2. CFD Mesh Generation

Once we have a geometric model representing the blood vessel of interest, we need to discretize the flow domain into elements for the simulation. This process is known as mesh generation.

Simvascular uses a finite-octree based tetrahedral mesh generator (TetGen). The idea behind finite-octree methods is to decompose a complex geometry into simpler pieces and then mesh the individual pieces using a mesh generation technique. After geometry is decomposed, Surface meshing is performed using projected 2D surface triangulation. Geometry is used to create the interior volume mesh, and 3D triangulation is used to complete the meshing process.

For the creation of our mesh, we set a global max element size of 1.2mm and volumetric and surface meshing options were selected.

In addition, boundary layer mesh is created to reduce computational cost without losing accuracy. 3 layers with a 0.8 decreasing ratio were added.

As a result, our mesh is formed by:

Number of nodes	117675
Number of Elements	689148
Number of Edges	43158
Number of Faces	28772

Figure 5.4: Mesh information

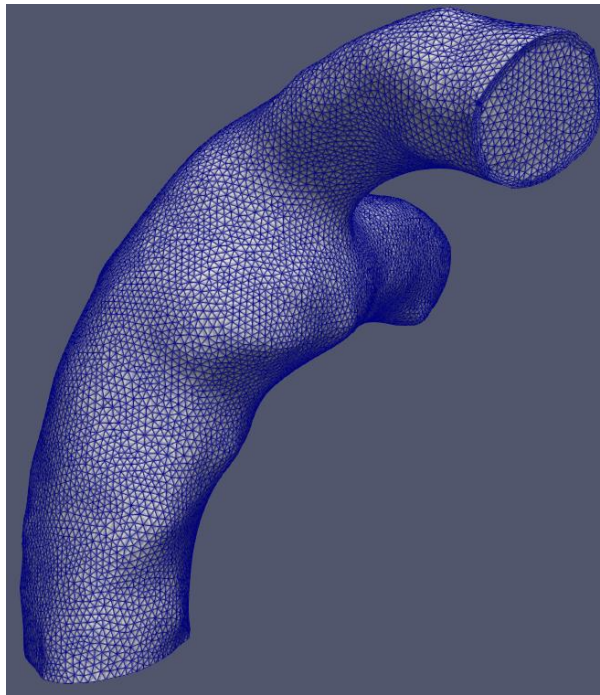


Figure 5.5: Mesh of the model

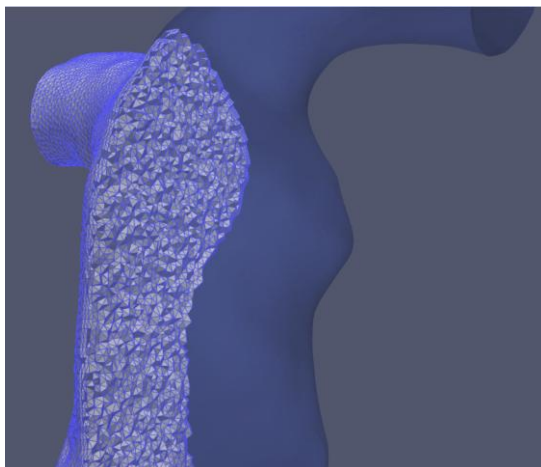


Figure 5.6: View of internal volumetric mesh

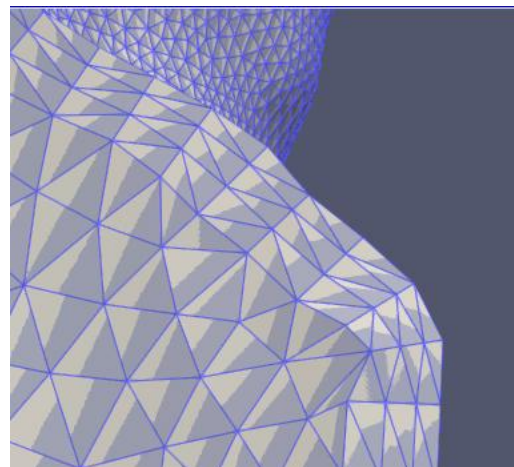


Figure 5.7: View of boundary layer mesh

5.3.3. Simulation files

In order to use the SimVascular solver, we need a number of certain files that are mandatory for running the program.

```
restart.0.1
geombc.dat.1

numstart.dat

solver.inp

bct.dat
```

Figure 5.8: Needed files to run the simulation

The most important files are *bct.dat* and *solver.inp*.

bct.dat: defines the inflow boundary condition both spatially and in time. The spatial definition is obtained through n_p point-wise velocity input blocks; n_p is the total number of nodes in the inlet face. The temporal definition is given by n_t input lines of the values at a certain position for n_t time points, t_1 to t_{n_t} .

Each block of data has, for each of the n_p spatial points, the following information:

- The coordinates of the point: x_1 x_2 x_3 and the number of time points n_t
- The list of velocity vectors v_x v_y v_z at time t

```
np nt
x1 y1 z1 nt nn
vx1 vy1 vz1 t1
. . . .
. . . .
. . . .
vxnt vynl vznt tnt
. . . .
. . . .
. . . .
xnp ynp znp nt
```

Figure 2.2.8: *bct.dat* structure

solver.inp: provides further info for flow solver, specifying parameters (density, viscosity, number of time steps, ...) that will be tackled in the boundary condition section.

In all the parameters that involves those two files, we are going to introduce standard data in the Simvascular interface with the only intention to run the *svPresolver* and obtain them, subsequently files will be modified with the porpoise of configuring the boundary conditions of the simulation.

Other files that won't be modified before running the simulation:

geombc.dat.1: containing mesh info and boundary conditions specified in the problem, created by *presolver*.

restart.0.1: containing initial conditions for our problem, created by *presolver*.

numstart.dat: initially contains the number 0. This number is used by the solver to identify the restart file that should be used as initial condition.

5.4. Boundary conditions

5.4.1. *bct.dat* – Inlet boundary condition

As explained in chapter 5.3.3, *bct.dat* defines the inlet velocity. In order to do the simulation, we need to have the same velocities that in the 4-D Flow image.

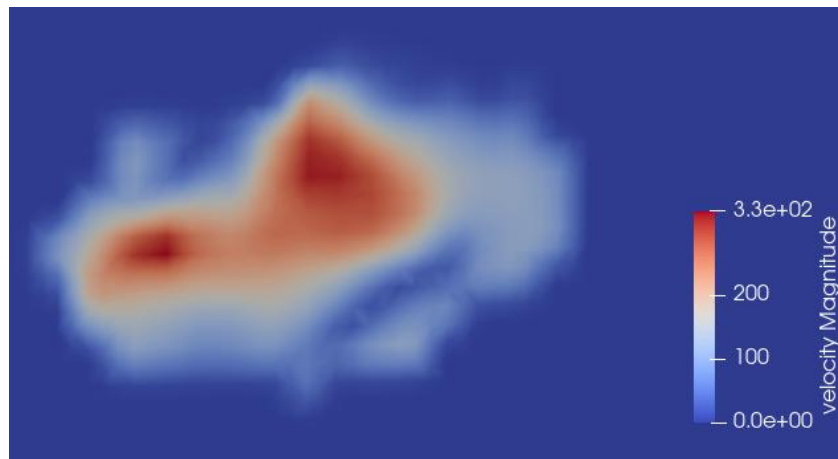


Figure 5.9: In vivo velocity distribution (mm/s) at time-step 0

To achieve that goal, it is necessary to transform *bct.dat* using Matlab. We are going to create a script with the intention of interpolating in vivo velocities in the CFD inlet points, and then, adding those interpolated velocities in *bct.dat* at every time-step.

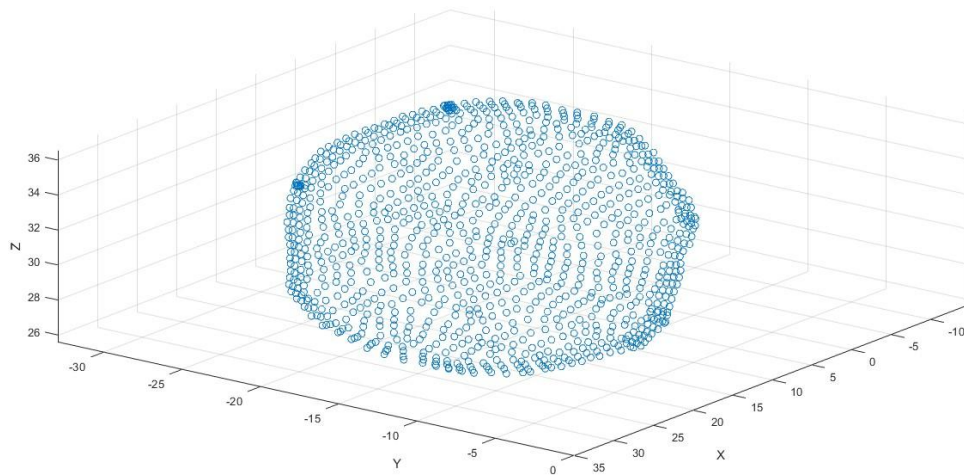


Figure 5.10: CFD inlet points

The result of the script is an updated bct.dat with 55381 rows. Following the bct.dat structure, the file has the velocity vectors (v_x v_y v_z) for each of the 51 time-steps at every inlet point of the CFD (1065 points).

5.4.2. Outlets Boundary condition

Resistance of the outlets is a relationship between flow and pressure of the form $p = p_0 + RQ$, where R is the resistance parameter that characterizes the downstream vasculature, p is the weakly prescribed pressure, Q is the flow rate passing through the face and p_0 is a “flag” that sets the boundary as a “weakly-prescribed pressure boundary”. This flag has a “zero” numerical value, so the total value of the pressure on that face is simply given by:

$$p = RQ$$

Assigning a constant pressure condition, and knowing the relative flow-rate distribution from 4-D data, leads us to the following resistances:

	Resistance ($g / mm^4 \cdot s$)
RPA	0.01
LPA	0.015

Figure 5.11: Outlets blood flow resistances

Those values will be added to the *solver.inp* file.

5.4.3. Wall conditions

Rigid Wall conditions will be assumed in the simulation, due to the difficulty of obtaining reliable data of the arterial wall properties. The main difference in the result of the simulation, compared with deformable wall, will be higher regional shear stress, with negligible differences in other flow patterns.

5.4.4. solver.inp

In this file we are going to indicate the rest of boundary conditions (blood density, viscosity and resistance values), and other necessary parameters to run the simulation (time-step size, number of time-steps between restarts, ...).

Density	0.00106 [gr/mm ³]	Fluid density
Viscosity	0.004 [gr/mm·s]	Fluid viscosity
Time Step Size	0.001	Time size of each step
Number of Timesteps between Restarts	50	Number of time steps between a new restart.. is saved. This values decides how often the complete status of the model is saved to disk.
Number of Force Surfaces	1	This line specifies the number of surfaces where we are going to collect traction in our model. Tractions are collected as a 'post-processing' step after the velocity and pressure fields are obtained

Step Construction	0 1 0 1 0 1 0 1	Non linear iteration sequence. It controls the non-linear iteration loop within the time step. The Navier-Stokes equations constitute a no-linear system of partial differential equations. Like any non-linear system, in order to find a solution for a given time step, we must undergo an iteration process to obtain a solution that reduces the residual (i.e., the error) as we iterate more and more. The 0 tells the solver to make a solve, the 1 to make an update of the solution. For example, a ten iterations solution is specified as default as a sequence of solve/update operations
Number of Resistance Surfaces:	2	Total number of surfaces with assigned resistance boundary condition
List of Resistance Surfaces	2 4	List of IDs (RPA and LPA) of surfaces with resistance boundary condition applied
Resistance Values:	0.01 0.015	Resistance values for the previously specified list of faces IDs

Figure 5.12: Non-default parameters in solver.inp

5.5. Simulation

Once we have all the boundary conditions and parameters of the solver set, we can proceed to run the simulation.

The simulation has been run, remotely, in the UPC-EEBE cluster, working on Linux shell. Connecting it via SSH server and UPCLink VPN, allowing working for home and transfer all files from/to our PC.

The used cluster has 16 processors, who run in parallel to reduce the simulation time. To run the simulation is necessary having the *svsolver* executable in the same folder we had all the mandatory files simulation files (see chapter 5.3.3)

While simulation is running we can visualize the following info, where:

a	b	c	d	e	f	g	h
17003	5.000E+00	2.565E-03	(-18)	7.234E-05	1.713E-03	< 4239-14 15>	[0 - 0]
17004	5.000E+00	1.662E-01	(0)	1.637E-03	2.138E-04	< 3384- 8 10>	[0 - 0]
17004	6.000E+00	7.564E-03	(-13)	7.506E-05	4.645E-06	< 4673-14 15>	[0 - 0]
17004	6.000E+00	2.906E-03	(-17)	9.154E-05	2.671E-03	< 6197-14 15>	[0 - 0]
17005	7.000E+00	1.655E-01	(0)	1.631E-03	7.563E-06	< 3384- 8 10>	[0 - 0]
17005	7.000E+00	7.536E-03	(-13)	7.117E-05	5.016E-06	< 4673-14 15>	[0 - 0]
17005	8.000E+00	3.315E-03	(-17)	7.015E-05	2.025E-03	< 2107-11 15>	[0 - 0]
17006	9.000E+00	1.655E-01	(0)	1.705E-03	1.363E-02	< 3384- 8 10>	[0 - 0]
17006	9.000E+00	1.032E-02	(-12)	1.032E-04	5.484E-05	< 4688-11 14>	[0 - 0]
17006	1.000E+01	4.318E-03	(-15)	1.341E-04	3.906E-03	< 4616-11 14>	[0 - 0]
17007	1.000E+01	1.676E-01	(0)	1.728E-03	2.828E-05	< 3384- 8 10>	[0 - 0]
17007	1.000E+01	7.558E-03	(-13)	7.798E-05	8.407E-06	< 4673-14 13>	[0 - 0]
17007	1.100E+01	2.950E-03	(-17)	7.403E-05	2.779E-04	< 4672-14 13>	[0 - 0]
17008	1.100E+01	1.665E-01	(0)	1.700E-03	1.484E-04	< 3384- 8 10>	[0 - 0]
17008	1.200E+01	7.458E-03	(-13)	7.917E-05	1.520E-05	< 4688-11 13>	[0 - 0]
17008	1.200E+01	2.866E-03	(-17)	8.215E-05	2.210E-03	< 5638-14 14>	[0 - 0]
17009	1.200E+01	1.660E-01	(0)	1.693E-03	1.894E-05	< 3384- 8 10>	[0 - 0]
17009	1.300E+01	7.298E-03	(-13)	2.677E-04	7.688E-03	< 4673-14 13>	[0 - 0]

Figure 5.13: Simulation while running on linux shell.

- **a:** Time step number – Each time step appears three times, this is because we are considering three non-linear iterations.
- **b:** CPU time seconds – This is counted since the analysis is launched
- **c:** Measure of the nonlinear residual – Indicates how accurate the solution is
- **d:** Logarithm of the residual change - provides a very good way of evaluating how well the solution is doing. If this number is very small and negative, then it is a good sign. An entry with the value “-10” means that you have reduced the residual by an order of magnitude from the beginning of the analysis, a -20, by 2 orders of magnitude, ...
- **e:** Entropy norm of the residual for the velocity field ($\max \Delta u/u$)
- **f:** Entropy norm of the residual for the pressure field ($\max \Delta p/p$)
- **g:** $\langle A - B | C \rangle$
 - **A:** block where the maximum residual happens (each block has 255 elements by default).
 - **B:** node in the block with the maximum error.
 - **C:** logarithmic measure of the ratio between the maximum residual and the average residual: want this number to be as small as possible: it will be an indicator of the spatial uniformity of the residual
- **h:** zero when using the default svLS.

That information is saved in the *history.dat* file, and, if it is necessary, can be analysed when the simulation is over.

The time needed to solve a complete cardiac cycle is around 10 hours (50.000 time-steps).

5.6. Post processing

When the simulation is finished, it needs to be post processed in order to have .vtu files that could be visualized in Paraview.

Running the *svpost* executable the selected “restart” files will be transformed in .vtu files, allowing too work on the solutions with Paraview.

6. Results

6.1. Flow rates

To obtain blood flow, we need to integrate the velocities, Paraview filters will be used to achieve that; same slice will be applied on both (in vivo and CFD) inflow and outflow. Then *integration* filter is going to be used on those slices, in order to have blood flows on every time-step, in the selected areas.

Once the integration filter is used, we export the results in a datasheet file with the objective to represent blood flow graphically.

LPA in vivo flow rate isn't represented due to the difficulty of obtaining the isolated data from 4-D image, their proximity to another blood vessel induce to higher values than expected (see figure 6.1)

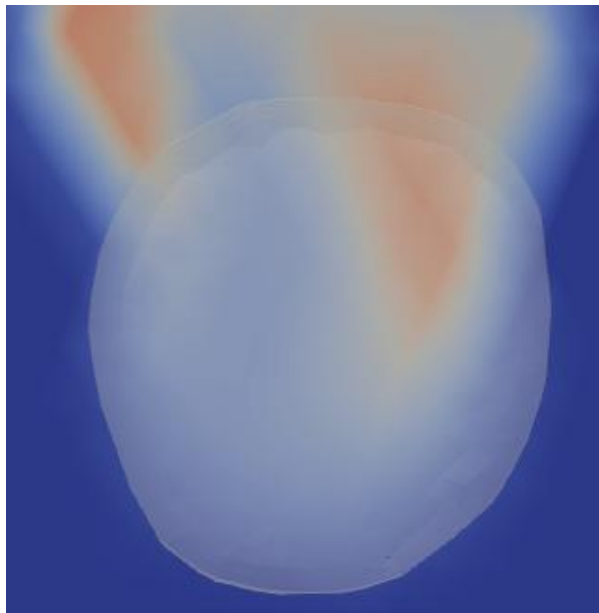


Figure 6.1: LPA outlet Surface overlay on 4-D image. Velocity field outside the outflow area can be appreciated

6.1.1. In vivo

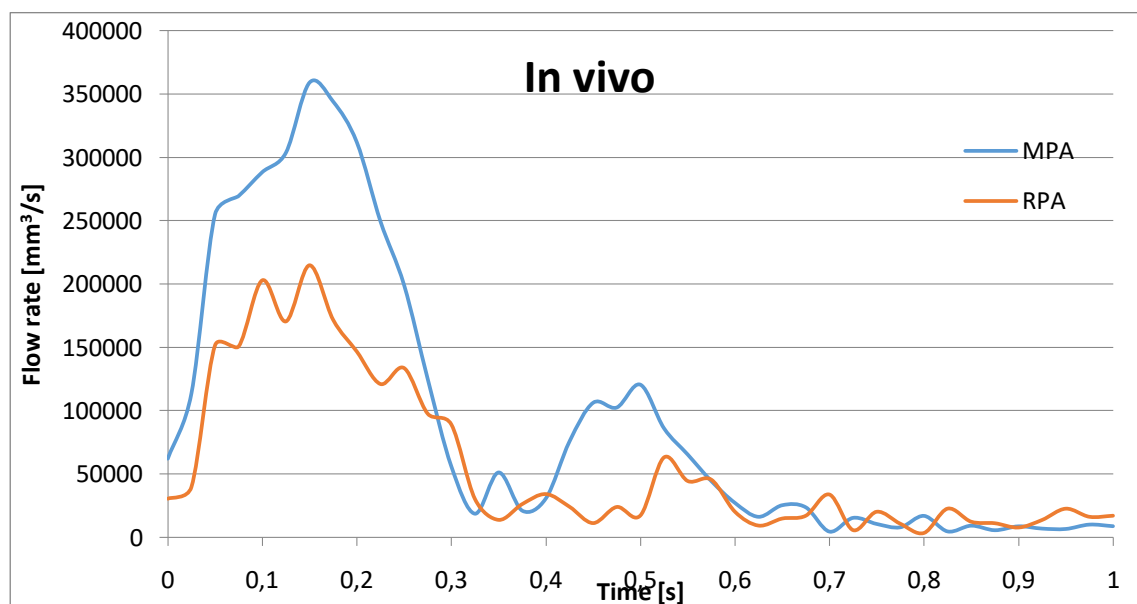


Figure 6.2: In vivo flow rate

Once we have the Inlet flow rate profile, we can locate four differentiated part in the waveform, (acceleration, peak, and deceleration). Those are the points of interest we are going to work on.

	In vivo				
	Time step[s]	MPA[mm ³ /s]	RPA[mm ³ /s]	LPA[mm ³ /s]	Flow Distr. (%)
Acceleration	0,05	254896	151605		59,48
Peak	0,15	358880	214829		59,86
Deceleration	0,25	199150	133657		67,11

Figure 6.3: In vivo flow rate results

This information, allows finding flow distribution between RPA/LPA. That distribution has been used to set up the resistances values.

We can see that RPA waveform is displaced 0.05s from the MPA flow rate and has some oscillations, before and after reach their peak. Despite that, both rate flows share the same waveform, as expected.

6.1.2. CFD

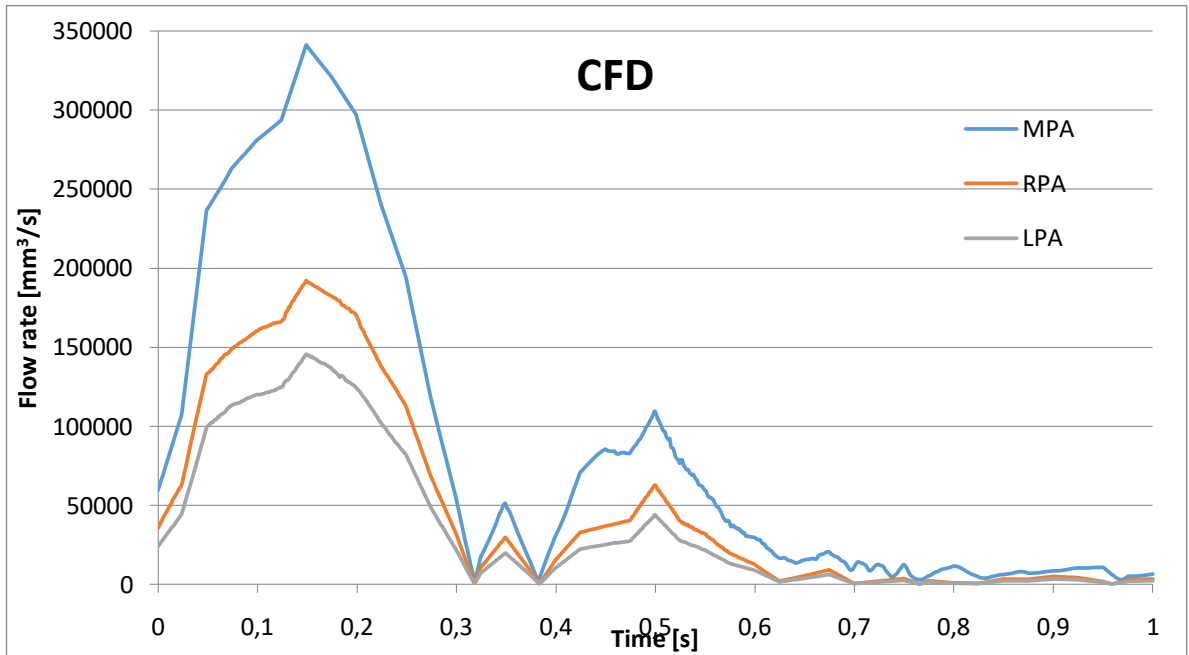


Figure 6.4: In vivo flow rate

As we did with in vivo data, we are going to locate the same points of interest, obtaining the following results (Figure 6.5):

	CFD				
	Time step [s]	MPA [mm ³ /s]	RPA[mm ³ /s]	LPA[mm ³ /s]	Flow Distr. (%)
Acceleration	0,05006	237860	133406	100076	56,1 – 42,1
Peak	0,1489	341197	192038	145559	56,3 – 42,7
Deceleration	0,2491	194713	112811	82063,8	57,9 - 42,1

Figure 6.5: CFD flow rate

We can see how all waveforms have fewer oscillations, compared to in vivo flow rates. Also, MPA, RPA and LPA share same form, having their peaks at same time-steps.

Instead, flow rates are slightly lower in their values compared to in vivo data.

6.1.3. In vivo vs CFD

In this chapter we are going to compare in vivo and CFD results. Only MPA and RPA are going to be analysed, because of the impossibility to calculate LPA in vivo outflow (see chapter 6.1).

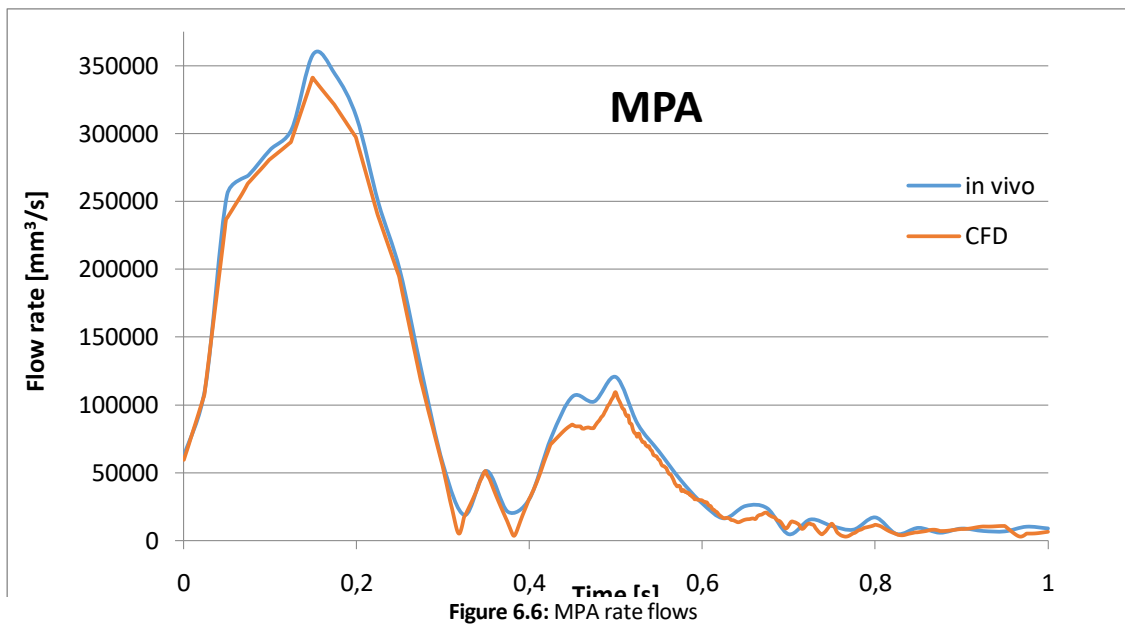


Figure 6.6: MPA rate flows

As we can see in Figure 6.6, inflow at CFD and in MRI data is basically identical. The main difference is the value in their peak. In CFD has a lower value, with around 5% percentage deficit compared to in vivo flow rate.

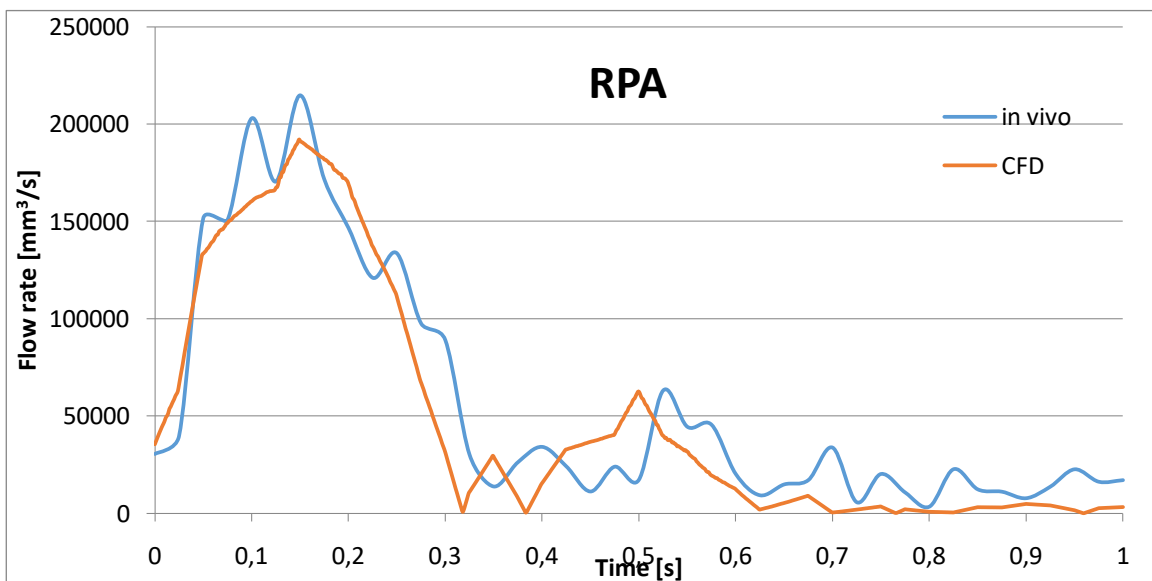


Figure 6.7: RPA rate flows

In contrast, differences in RPA are more obvious (see figure 6.7), the same displacement in the waveform that in vivo RPA has with in vivo MPA flow, still appearing compared with RPA CFD. Also, oscillations aren't present in CFD RPA.

Patron we described with the MPA peak values of in vivo – CFD, also has presence in RPA. With a higher difference of the 11%, between CFD peak and in vivo peak.

6.2. Velocity profiles

In this chapter, velocity profiles are going to be compared in each point of interest labelled in chapter 6.1.

In order to observe velocity distribution on the PA, we are going to use slice filter, the plane used to do the slice is going to be the same in CFD simulation and in invivo data. Doing that, we are going to be able to compare them.

6.2.1. Time step 0.04 – Acceleration phase

First velocities we are going to compare are the inflow velocities. Compare them will help us to validate the bct.dat modifications we did (explained in chapter 5.4.1).

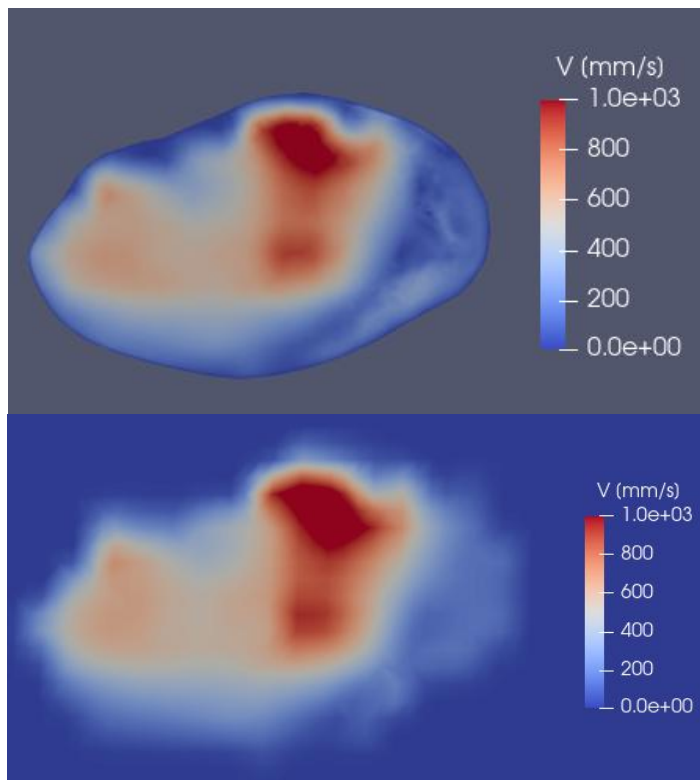


Figure 6.8: CFD vs In-vivo inflow at time-step 0.04s

As can be seen in figure 6.8, In-vivo and CFD inflows are very similar, as expected.

When the inflow condition has been validated, we can compare the velocity distribution in RPA/LPA.

In figure 6.9, is it visible that even having very similar flow-rate values (chapter 6.1), the velocities are distributed differently between CFD simulation and 4D image data.

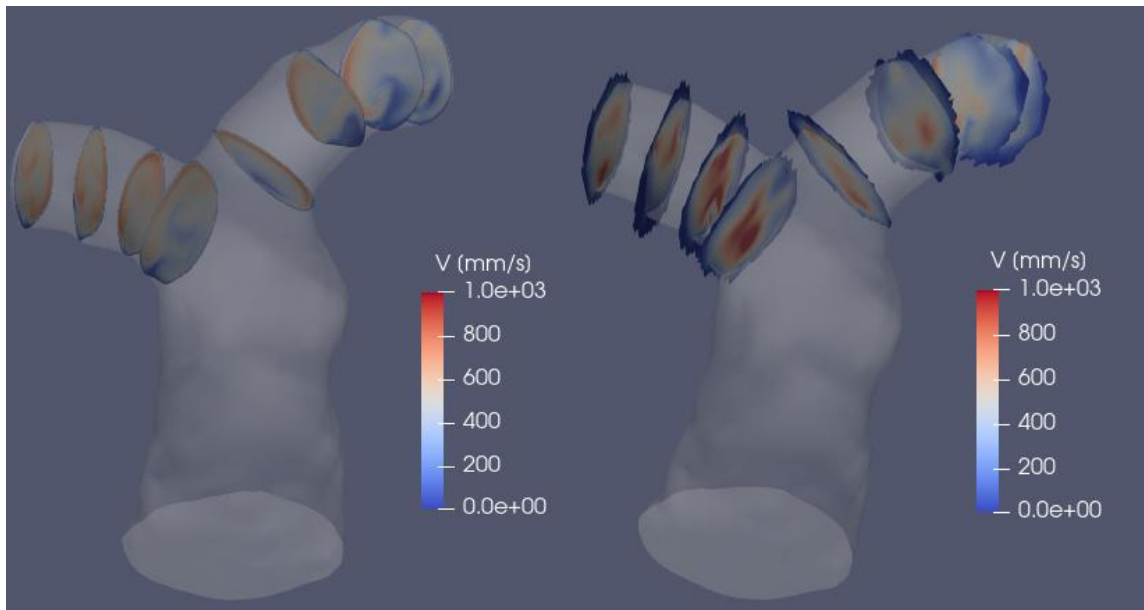


Figure 6.9 : Velocity field at time-step 0.04s (Left: CFD; Right: in-vivo)

In the in-vivo data the velocity is concentrated in fewer points, and in general maximum velocities are located in the geometrical centre of the RPA/LPA. Instead, CFD velocities have a more “homogeneous” distribution, and vortex can be easily observed.

6.2.2. Time step 0.12 – Peak phase

At time step 0.12, in the peak of the flow waveform, inflows stills with the expected values. How we can see in figure xx, in vivo data and CFD solution are basically identic.

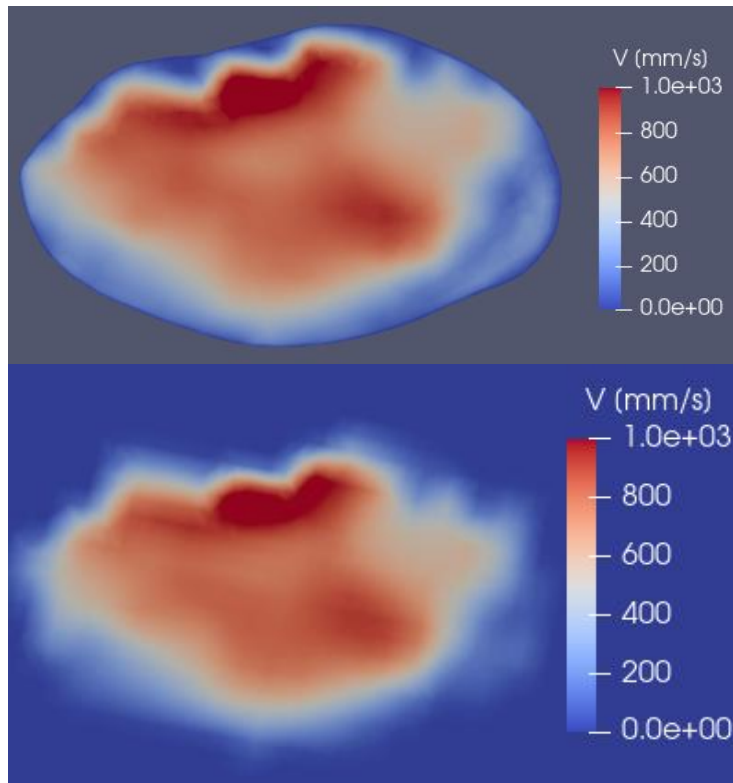


Figure 6.10: CFD vs In-vivo inflow at time-step 0.12s

For better visualization, in this section, RPA and LPA will be compared for separated.

In RPA, we can observe more similarities between CFD and in vivo data, but in vivo velocities still being more concentrated.

In the bifurcation nearest slice we can clearly view same vortex structure in both (CFD and in vivo) images. Those turbulences are typical in blood vessel bifurcation as PA.

Also in the other RPA slices, we can see similarities in the way max velocities are distributed.

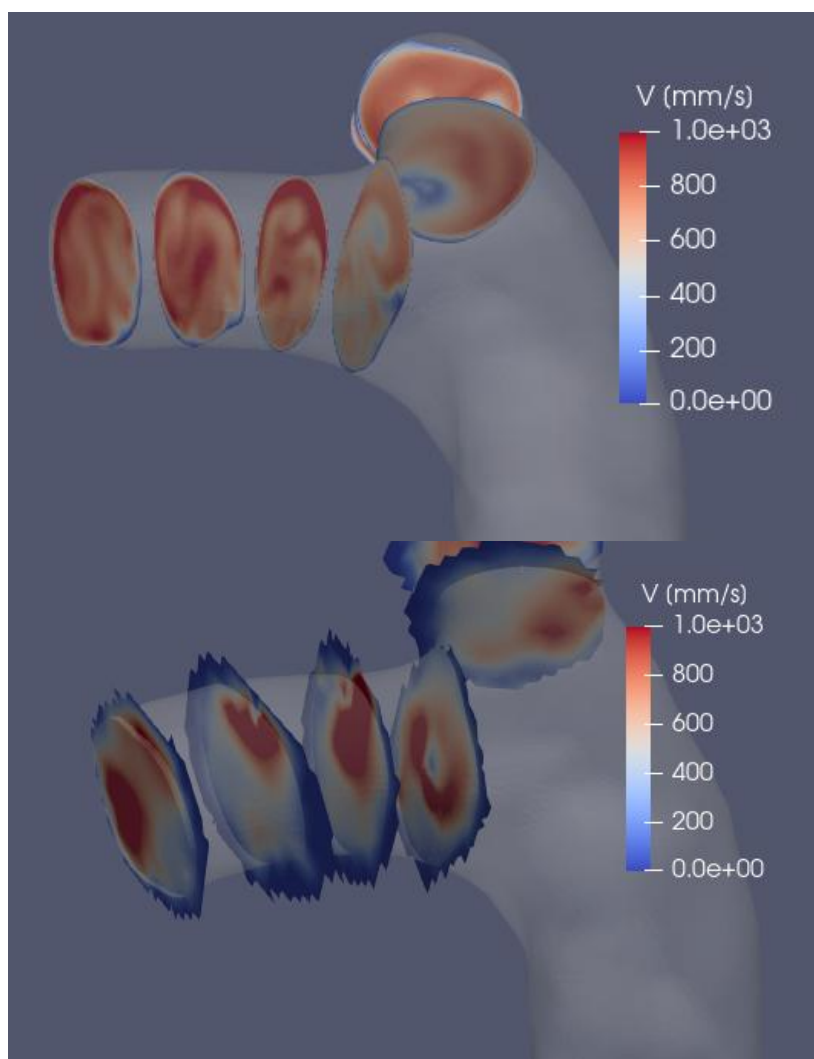


Figure 6.11: RPA velocity distribution at time-step 0.12s. CFD vs in-vivo

Those same similarities are present in LPA. Turbulence near the bifurcation isn't visible in the 4D-image, but velocity distribution has a good correlation between CFD and in-vivo. Maximum velocities are located in the same areas and the flow structure could be take it as "equal" despite de low resolution of in-vivo data.

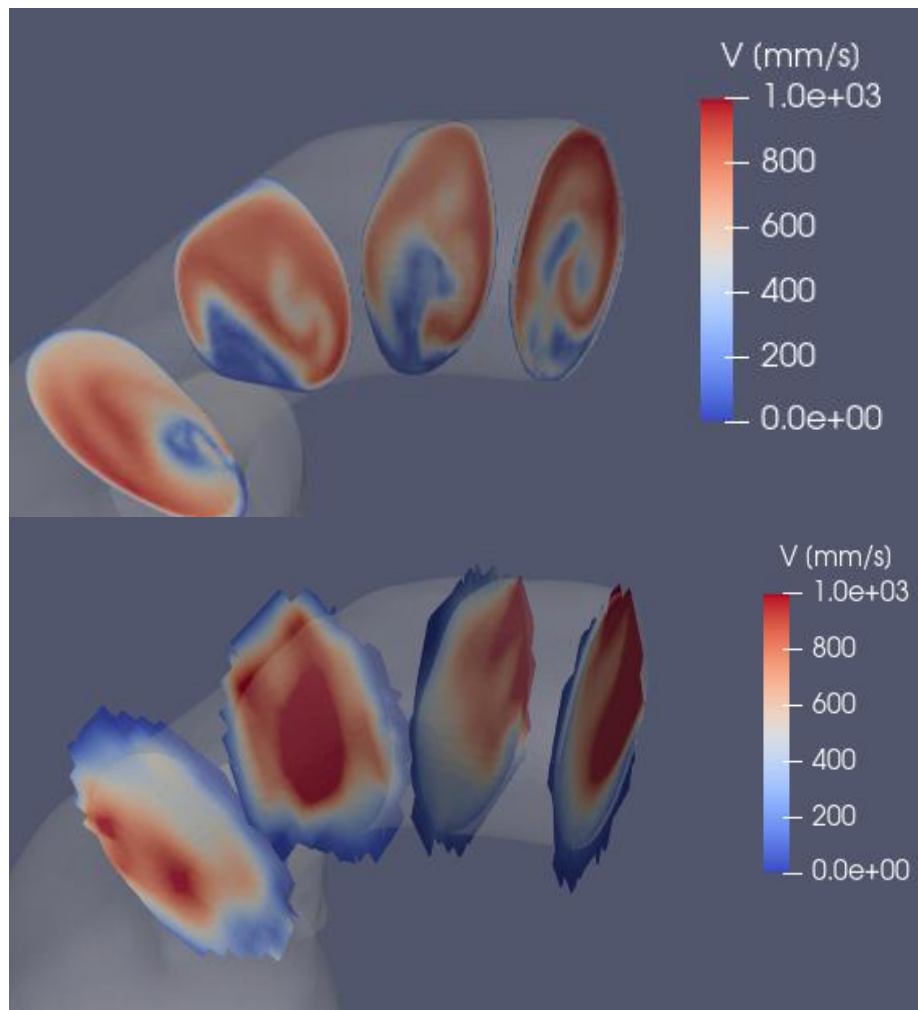


Figure 6.12: LPA velocity distribution at time-step 0.12s. CFD vs in-vivo

6.2.3. Time-step 0.20 – Deceleration phase

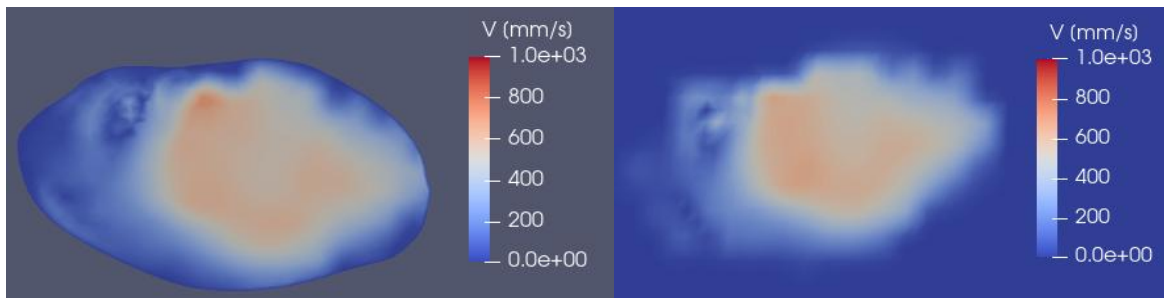


Figure 6.13: CFD vs In-vivo inflow at time-step 0.2s

Last visually analysed time-step continues with the exact correlation between CFD and in vivo inlet velocities. Confirming the changes we did to bct.dat are correct, and validating the Matlab script used to change the file, allowing using it in future cases.

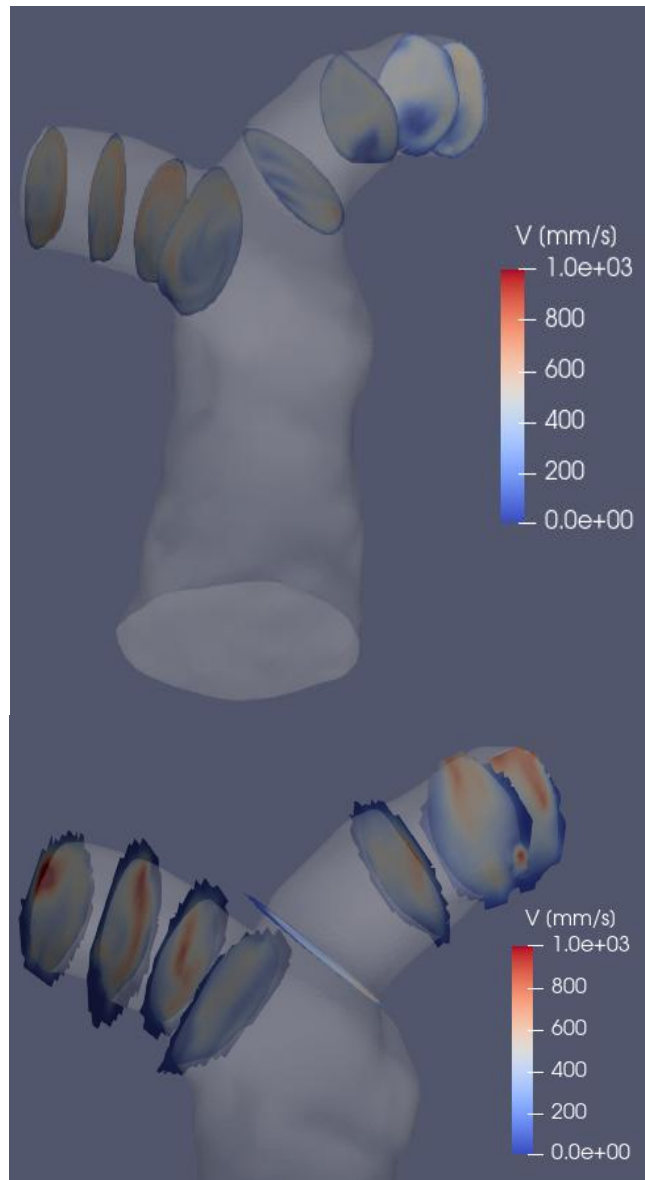


Figure 6.14: Velocity field at time-step 0.2s

In this case, comparing both cases implies some difficulty, due to the lower values at the deceleration zone, and the in vivo tendency to having the velocities concentrated. Despite that difficulty, we can see some flow structures are replicated in both cases. For example, in the RPA slice nearest to the bifurcation and in the LPA outlet.

6.3. Q-criterion

Coherent vortical structures in the flow can provide valuable understanding of the flow field in a variety of cases, but visualization of unsteadiness in a flow field can be difficult to convey and illustrate.

Q-criterion [11] is used to visualize those vortical structures. Q criterion defines vortices as areas where the vorticity magnitude is greater than the magnitude of the rate of strain.

This parameter can be visualized in Paraview selecting two filters. The first used filter is *Gradient*, which estimates the gradient vector at each point or cell. It operates on any type of vtkDataSet, and the output is of the same type as the input. For unstructured grids, the gradient is computed with the cell derivatives. It allows computing Q-criterion directly.

Once we have Q-criterion, *Contour* filter is applied. These filter, generate isolines or isosurfaces using point scalars, and help us to visualize Q-criterion and their structures. The value range of the isosurfaces will be set up at 20.000 in order to compare vorticity at different time steps.

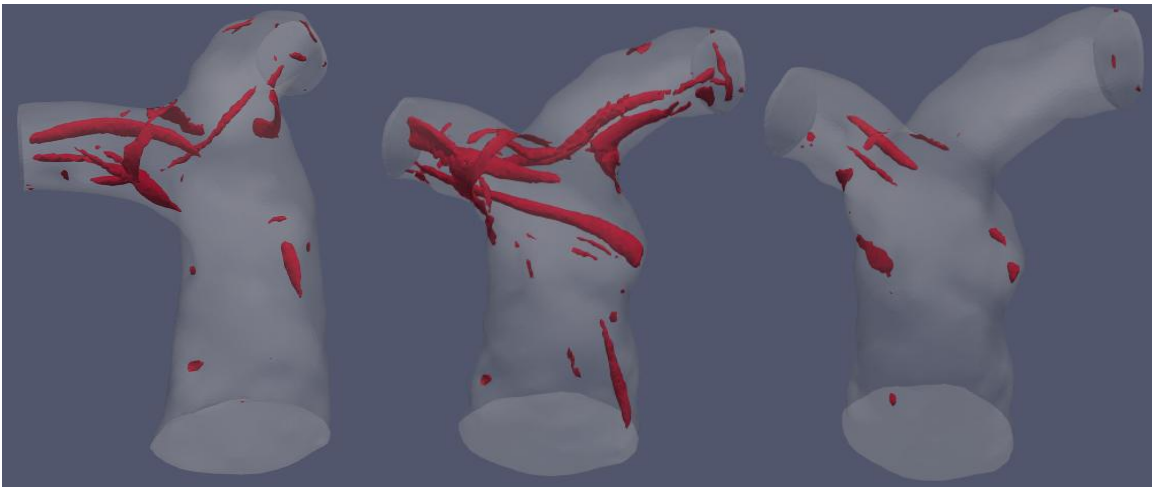


Figure 6.15: Q-criterion representation at time-step 0.04s(Left), 0.12s (Centre) and 0.20s (Right).

As seen in figure 6., vertical structures tend to raising up when higher velocities are involved, having maximum systolic vorticity at time-step 0.2s (systolic peak).

At time-step 0.04s some vortex are mainly represented in RPA, where velocities are higher compared to LPA.

At time-step 0.12s, as mentioned, we have maximum vorticity, having clearly represented vortex in MPA, RPA and LPA.

At time step 0.20s, compared to other time-steps, vorticity is residual only having little turbulences at RPA.

The Q-criterion results obtained in the simulation follows the typical structures presented in pulmonary arteries. Elongated, pencil-like structure protruding predominantly into de RPA, while being quickly dissipated in the initial tract of the LPA [4][14].

6.4. Wall Shear Stress - WSS

Shear stress is a frictional force tangential to the direction of a flowing fluid, the force of which is directly related to the fluid's viscosity shear stress.

Ass seen in other flow parameters, the maximum values of the WSS appear at the systolic peak (time-step 0.12s).

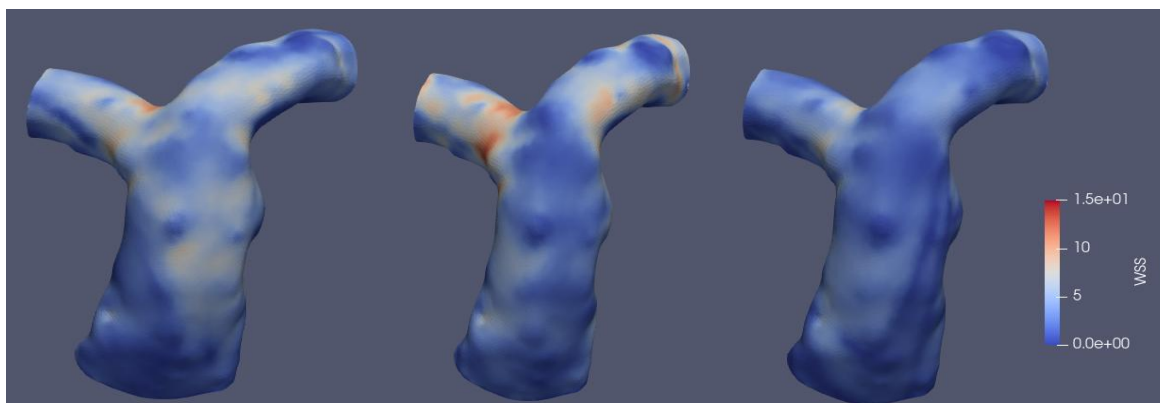


Figure 6.15: WSS[Pa] at time-step 0.04s(Left), 0.12s (Centre) and 0.20s (Right)

Also, we can observe where we can find higher WSS values are in the RPA/LPA near where the bifurcation begins. As mentioned in chapter 5.4.3, values are higher compared to the standards [15], as a consequence of rigid wall condition.

Conclusions

In this project, the fluid dynamics in a pulmonary artery have been analysed. The computational resolution of the Navier-Stokes equations has been carried out through the open source program SimVascular. In order to set the boundary conditions, in vivo data had to be previously analyzed, once all the useful information from in vivo data (patient-specific PA geometry, inflows, outflows, ...) are obtained, has to be processed with the objective to could use it as BC's in SimVascular, a program that needs a very specific inputs to work. The developed Matlab scripts used to add in vivo inflow during all the cardiac cycle into SimVascular solver files, could be used in the future to adapt those files in other patient-specific cases.

Once the simulation has been run, it has been found that the mathematical model and the boundary conditions used were valid. It has been observed that blood flow and its distribution were very similar (Simulation-in vivo) with differences around a 5% of the total inflow, and 2% in the flow distribution (RPA/LPA). Also some vorticity structures are shared between in vivo and simulation can be seen on the velocity field distribution, where similar structures appear at the same time-step and location. These vortices are obvious in the visualization of the Q-criterion, where it has been possible to observe the appearance of vortex structures that forms into the MPA inner wall and gradually elongate, especially to the RPA.

Concluding that the mathematical model used for the finite element analysis allows to efficiently simulate the blood flow in the PA, thus simulations will helps to have a better understanding of blood flow parameters for different condition patient, allowing to relate some flow features with determined heart pathologies.

A part from the main objective, simulation and their validation, and from typical blood flow features that were necessary to learn, in order to do the project. Further knowledge has been acquired, as working with all the software involved in the resolution of this simulation as SimVascular (plus running it on Linux console), Paraview, Matlab, and working on a cluster on remote.

Economic Analysis

This economic analysis has two differentiated parts: Material used and human resources needed to develop the project.

Materials

In this section appear all the used materials that have a cost, though the University provided them without cost.

Material	pcs	Unitary cost	Total cost
MRI Scan	1		250,00 €
Laptop Acer Aspire V5 - 552G	1		650,00 €
Matlab R2022a - Academic Use	1		250,00 €
Cluster 16-procs	80	1,08€/h	86,40 €
Microsoft 365 License	4	9,66€/month	38,64 €
TOTAL			1,275.04 €

Human resources

Human Resources	pcs	Unitary cost	Total cost
DIRECTOR	50	60€/h	3,000.00 €
Student	600	8€/h	4,800.00 €
TOTAL			7,800.00 €

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