Relationship between flow patterns, energy efficiency and shape variations in the healthy pulmonary arteries via patient-specific numerical simulations

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L'étude a utilisé la simulation numérique des fluides pour évaluer l'artère pulmonaire (AP) sous diverses conditions d'entrée, en se concentrant sur l'énergie cinétique tout au long du cycle cardiaque. Des schémas d'écoulement distincts ont été observés, en particulier pendant les phases d'accélération et de pic systolique. L'analyse de l'hélicité et les structures tourbillonnaires ont mis en évidence les interactions complexes influencées par la courbure de l'AP. Sa performance a été évalué en comparant l'énergie cinétique moyenne avec les pertes énergétiques, mettant en avant les limitations de l'étude. La paramétrisation des modèles 3D d'AP a permis de souligner une éventuelle corrélation entre courbure de celle-ci et sa performance.

Mots-clefs : artère pulmonaire, dynamique des fluides computationnels

The study utilized computational fluid dynamics to assess the pulmonary artery (PA) under diverse inlet conditions, focusing on kinetic energy throughout the cardiac cycle. Distinct flow patterns were observed, especially during acceleration and systolic peak phases. Helicity analysis and vortical structures highlighted the intricate interactions influenced by the PA's curvature. Its performance was assessed by comparing average kinetic energy with energy losses, highlighting the study's limitations. Parameterization of 3D PA models highlighted a possible correlation between curvature and performance.

Keywords : pulmonary artery, computational fluid dynamics

1. General context

Computational Fluid Dynamics (CFD) simulation has been pivotal in various industries and has recently gained traction in the biomedical realm, especially regarding blood flow dynamics in the cardiovascular system. Although systemic circulation has been extensively researched, the study of blood flow dynamics in the pulmonary arteries using CFD remains nascent. The nuanced flow patterns and vessel geometry necessitate refined computational models for accurate simulations. CFD studies in medicine show immense potential, promising insights into disease progression, optimizing medical tools, and aiding in personalized patient care.

The primary aim of the presented research is to craft and validate a methodology for simulating Pulmonary Artery (PA) blood flow in healthy individuals. By utilizing Statistical Shape Analysis (SSA) of the PA, the study intends to mathematically characterize the shape variations between the different subjects and compare it with the studied hemodynamic parameters. The comprehensive characterization of blood flow dynamics in healthy subjects will help to understand the normal blood dynamics and therefore pave the way for pinpointing anomalies in patients. The research process includes software adaptation, clinical imaging data preprocessing, simulations, and post-processing, with automation considered for certain stages.

2. Introduction

2.1. Cardiovascular system

The pulmonary artery (PA) plays a vital role in the cardiovascular system, transporting deoxygenated blood from the heart's right side to the lungs for oxygenation (fig. 1). Originating from the heart, the main pulmonary artery (MPA) branches into the right (RPA) and left pulmonary arteries (LPA), which subsequently lead to smaller capillaries for gas exchange. This T-shaped branching structure enables the essential oxygen-carbon dioxide exchange, with the PA, a short vessel of about 5cm, operating efficiently under low pressure and high flow rate.

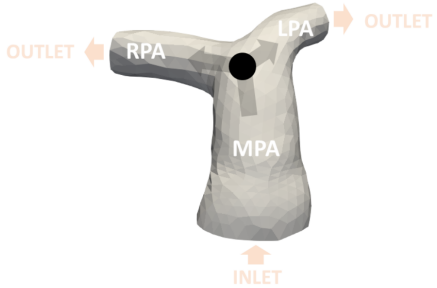

Figure 1 : Pulmonary artery T shape as shown by a segmented 3D model

The PA's function complements the broader cardiovascular system, wherein the heart's chambers and valves regulate blood circulation. After the right atrium receives deoxygenated blood, it's sent to the right ventricle and then through the pulmonary artery to the lungs (fig. 2). Following oxygenation in the lungs, the rejuvenated blood returns to the heart and is distributed throughout the body. This continuous circulatory process is fundamental for body health, emphasizing the importance of understanding the PA and cardiovascular system for addressing related diseases and promoting overall health.

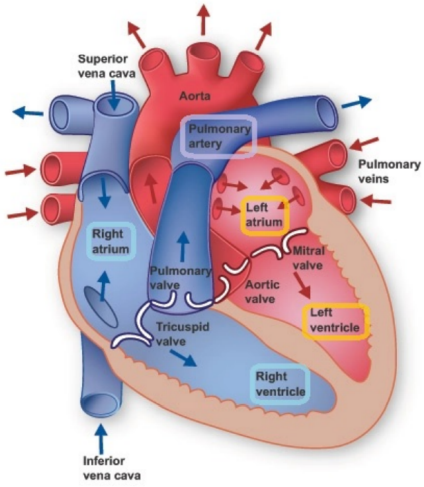

Figure 2 : Anatomy of the heart (simplified version)

2.2. Blood flow dynamics

The cardiac cycle, a fundamental process in the cardiovascular system, consists of two phases: diastole and systole. During systole, which is marked by three key stages—acceleration, peak systole, and deceleration—the heart contracts and pumps blood to the body. In the acceleration phase, the right ventricle contracts, causing pressure to rise, leading to the opening of the pulmonary valve and the ejection of blood into the pulmonary artery (PA). Peak systole represents the moment of maximum contraction and blood ejection, while deceleration occurs as the heart begins to relax. During systole, blood velocity in the PA increases significantly, reaching a maximum flow rate of 900 mm/s (Re = 3400, D = 27 mm) [1], playing a crucial role in efficient blood pumping and maintaining proper blood pressure.

Blood properties, especially its viscosity, depends on factors such as shear stress and vessel diameter [2]. Although blood is a complex non-Newtonian fluid, in the context of computational fluid dynamics (CFD) simulations of the PA, it is often simplified as a Newtonian fluid due to the large diameter of the PA, which limits

the effect of viscosity changes [2]. This simplification enables more straightforward numerical calculations.
The flow dynamics within the pulmonary artery have garnered limited knowledge, especially in healthy individuals. Recent advancements in imaging techniques and computational modelling have provided valuable tools for exploring these flow patterns, with studies revealing vortical structures and variations in flow patterns in different pulmonary artery segments [1, 2, 3, 4]. However, there is still much to learn about normal flow patterns, especially in the context of various physiological and pathological conditions. Additionally, the curvature of the pulmonary artery contributes to the development of Dean vortices [4], which impact flow behaviour and add complexity to pulmonary artery hemodynamics, highlighting the need for further research in this area to gain a deeper understanding of these vital processes.

2.3. Imaging methods

Magnetic Resonance Imaging (MRI) stands out as the primary imaging technique for this research. MRI captures detailed 3D images of the body's internal structures using strong magnetic fields. Specifically, the 4D-flow MRI method visualizes the blood flow within the pulmonary artery over time, offering high-quality, dynamic, and non-invasive insights crucial for CFD simulations. MRI's ability to provide isotropic three-dimensional resolution allows clinicians to visualize vessels from various perspectives, contributing essential data for CFD simulations of vascular dynamics.

2.4. Computational Fluid Dynamics

The methodology for applying Computational Fluid Dynamics (CFD) to medical contexts, especially blood flow modelling in the human body, involves seven stages as highlighted by Morris et al [5]. The process starts with obtaining high-resolution medical images like MRI or CT scans. These images are then segmented and reconstructed into a 3D model using specialized tools. The model undergoes spatial and temporal discretization (or meshing), setting the stage for simulation accuracy and computational resource allocation. Physiological boundary conditions (BCs) are then established based on patient data or assumptions. With these elements in place, the physical parameters are defined, allowing the CFD solver to compute the necessary fluid dynamics equations. Finally, post-processing extracts and presents the relevant results from the simulation.
The Navier-Stokes equations form the core of CFD simulations, describing the motion of viscous fluids. This equation is simplified to express the conservation of mass, momentum, and energy in a fluid domain. In pulmonary artery (PA) flow simulations, these equations approximate blood flow patterns within the vessel, guided by conservation principles.

Various assumptions are made, including that blood follows Newton's law, is incompressible, has constant viscosity, tissue elasticity is neglected, and there is no-slip at vessel walls. Inflow rates are specified from upstream, and outflow conditions at downstream are defined as resistive. Therefore, the relationship between flow rate (Q) and pressure drop (ΔP) across a purely resistive element is described using Ohm's law.
The finite element method (FEM) is chosen to numerically solve partial equations, using SimVascular. FEM discretizes the domain into finite elements, proving suitable for addressing mathematical complexities.

3. Materials and methods

3.1. Overview of the methodology

The methodology employed in this study consists of several key steps aimed at understanding and analyzing the pulmonary artery's flow dynamics:

1. Preparation of CFD Simulation: This initial step involves processing anatomical models and defining necessary parameters and boundary conditions. It also integrates MRI data as an inlet condition and facilitates data visualization.
2. Execution of SimVascular Simulations: After preparation, simulations are run using the SimVascular software on a cluster, allowing for the numerical modelling of blood flow in the pulmonary artery.
3. Processing of Simulation Results: Once simulations are completed, the results are processed to extract relevant quantities of interest. Various tools, including Paraview and MATLAB, are used for data processing and visualization.
4. Statistical Shape Analysis (SSA): In parallel with CFD simulations, a separate SSA study is conducted using Deformetrica. This step allows to generate different mathematical parameters (modes) characterizing each PA shape, using as a reference an average model.
5. Correlation Analysis: The CFD and SSA results are combined for a correlation study. This analysis explores relationships between various parameters obtained during CFD result processing, shedding light on the interplay between flow dynamics and pulmonary artery shape.

3.2. Clinical data

This study involves a population of 35 healthy adults aged between 19 and 45 years. The data was obtained through Cardiovascular Magnetic Resonance (CMR) using a 1.5 T scanner with high spatial resolution (2.5 mm isotropic) and temporal resolution (24 ms mean). The CMR technique allowed for the acquisition of time-resolved three-dimensional velocity data, commonly referred to as 4D-flow. The

dataset is initially organized into three separate files: one contains velocity information in MATLAB Data format (comprising three matrices: Vx, Vy, and Vz, each of size 160x160x160), another stores acquisition-related properties in DICOM[1] format (providing details like the coordinates of the local reference frame, orientation vectors, and acquisition step), and the third is an STL[2] file containing the geometry of each pulmonary artery (PA) extracted from the CMR scans. This comprehensive dataset forms the basis for the subsequent computational fluid dynamics (CFD) simulations and statistical shape analysis (SSA) conducted in the study.

3.3. Model processing

In the context of this study, the raw surface representation of pulmonary artery (PA) models often exhibits irregularities, particularly in the upstream and downstream sections. To prepare these models for computational fluid dynamics (CFD) simulations and statistical shape analysis (SSA), a processing step is necessary. Manual processing with MeshMixer is chosen, focusing on truncation and smoothing, followed by integration into SimVascular for further tasks.

3.4. Discretization

The Courant-Friedrichs-Lewy (CFL) condition is employed to estimate an appropriate time step size, preventing convergence issues caused by excessively large or small-time steps. The integration schema used is the implicit. The time step size is determined based on parameters like the maximum speed of incoming blood flow and the mesh size.
The maximum speed of the incoming blood flow is assumed to be approximately 1800 mm, with a safety factor of 1.4, resulting in a considered speed of 2520 mm/s. The Global Mesh Edge Size (GMES) is a parameter used to quantify mesh refinement. The choice of GMES depends on the specific simulation's purpose, with finer meshes used for in-depth analysis (GMES=0.7) and coarser ones for global results (GMES=1.5). Assuming a 1s cardiac cycle, the total number of time steps would be 4000 or 1600, depending on the time step size considered.

In CFD simulations, complex domains are discretized or meshed into finite subdomains or elements. This step is essential for performing numerical calculations of partial differential equations, such as the Navier-Stokes equations. SimVascular uses TetGen, a tetrahedral mesh generator, as its default tool for mesh generation.

[1] “Digital imaging and communications in medicine” file is a recognized worldwide standard for the exchange of medical images.
[2] “Standard Tessellation Language” file describes an unstructured triangulated surface.

3.5. Boundary conditions

Boundary Conditions (BC) are paramount in CFD simulations to ensure accurate representation of the real-world scenario. The walls of the vessels in this study are considered rigid with a no-slip condition, meaning zero velocity at the wall. It is important to note that the inflow BCs are driven by in-vivo imaging data. Following the findings of Capuano [1], the latter allows to consider the compliance and downstream impedance. In other words, the usage of patient specific inlet conditions would reflect the fluid-structure interactions of the PA and the downstream vessels. Therefore, the implications of the rigid PA walls assumption may be secondary [6].

This inflow condition is implemented using a specialized script post SimVascular configuration. Outflow conditions, on the other hand, employ a Windkessel RCR model [7]. The resistance parameters are tuned to provide a normal flow split, i.e., 55% of the flow to the right side and 45% on left side [1, 8].

3.6. Patient-specific velocity field processing

The script developed for this project is a crucial component of the workflow, facilitating the conversion and integration of raw MRI data into SimVascular. Its development has been a major focus, requiring extensive effort to overcome resource-intensive challenges. One significant challenge was the conversion of MRI data into a format compatible with SimVascular. This necessitated a deep understanding of both MRI data acquisition and SimVascular software to bridge the gap between real-world data and computational fluid dynamics (CFD) simulations.

The script handles the conversion, processing, and integration of MRI data into SimVascular, ensuring proper formatting and compatibility with the simulation software. This integration allows for a more accurate representation of patient-specific hemodynamics in the pulmonary artery. While the detailed development of the script is not covered here, its key functionalities include creating a velocity interpolation function and assigning inlet conditions based on in-vivo velocity fields.

The velocity interpolation function is a fundamental component that accurately represents patient-specific information in CFD simulations. It utilizes various datasets, such as DICOM coordinate matrices, MAT[3] velocity matrices, and processed STL files. The script initializes with user-defined settings, loads velocity matrices, extracts acquisition parameters, creates coordinate matrices, performs

[3] MAT file is a MATLAB® file that store workspace variables

spatial restrictions, handles formatting differences, and ultimately generates the interpolation function.

Assigning inlet conditions based on in-vivo velocity fields involves modifying the BCT (boundary condition table) file generated by SimVascular. The script reads this file, extracts simulation parameters and coordinates, creates a new matrix with formatted data, performs velocity interpolation for each inlet point and time, and overwrites the old BCT file with the modified data.
Furthermore, the script generates VTK (Visualization Toolkit) files compatible with Paraview, allowing for post-processing and visualization. It begins by generating a tetrahedral mesh from the 3D model (STL file) and then determines velocities for each node of the volume mesh at each time step using the interpolation function. Finally, it generates and saves VTK files for each time step, ensuring compatibility with Paraview for in-depth data analysis and visualization.

3.7. Statistical shape analysis

Statistical Shape Analysis (SSA) evaluates geometric variations in anatomical structures, emphasizing shape attributes over size, and seeks correlations between shape variations and functional properties. In relation to pulmonary artery's Computational Fluid Dynamics (CFD) simulations, SSA discerns the impact of artery shape on blood flow dynamics. A methodology for generating results employs scalar "modes" to describe different initial geometries relative to an average reference shape. Creating a Statistical Shape Model (SSM) encompasses aligning shapes, computing an average shape, and using Principal Component Analysis (PCA) to pinpoint main shape variation modes. These modes, ranked by significance, capture the bulk of shape variability. Variations in each mode are analyzed by sequentially adjusting one mode while others remain fixed, elucidating each mode's contribution to overall artery shape differences.

3.8. Post-processing

To facilitate the interpretation of results across the wide range of cases studied, scalar quantities have been developed. These scalar quantities condense the 4D information from the simulations into single values, removing the complexities of time and space dimensions. Scalar quantities are utilized to distill complex simulation data, providing a streamlined interpretation by eliminating intricacies related to time and space dimensions by integrating over these two. This makes it easier to identify trends, understand relationships between variables and compare across different scenarios. In the project, Paraview macros automate tasks like data extraction and export, which are then analyzed in MATLAB. With its robust mathematical capabilities, Matlab, combined with Paraview, ensures efficient data processing

and a deeper examination of Computational Fluid Dynamics (CFD) simulation results.

On the other hand, 4D analysis (time and space) provides a comprehensive understanding of fluid dynamics, with tools in Paraview enabling detailed examination of parameters like flow patterns and vorticity. Due to the vast number of cases, an efficient filtering process, grounded on mean kinetic energy curves, is employed to sift through data and identify anomalies. Cases that significantly diverge from expected patterns are earmarked for further scrutiny or possible omission, guaranteeing the consistency of analysis. In-depth evaluations, such as the correlation between kinetic energy at the inlet and the system's global kinetic energy, further underscore the influence of input conditions on the entire system. Manual validation is also undertaken for selected cases to affirm their pertinence.

3.9. Quantities

Scalar quantities have been developed to analyze simulations, eliminating the complexities of time and space. These scalar values offer a convenient way to compare and simplify intricate datasets by neglecting time and space variability.
Energy losses (Elosses) in the pulmonary artery during a cardiac cycle (CC) shed light on the energy balance, with two methods being employed to measure these losses: control-volume analysis and quantification based on viscous fluid interactions. The second method have been employed to facilitate the automation the large dataset processing:

$$E_{losses} = \int_{CC}\int_{V} \frac{1}{2}\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2 dV dt,$$

Energy losses and the mean energy over a CC are computed as follow:

$$E_{losses} = \frac{1}{V}\int_{CC} P_{losses}(t)dt \quad [\frac{J}{m^3}]$$

$$P_{losses}(t) = \mu \int_{V} 2(\frac{\partial u'}{\partial x})^2 + 2(\frac{\partial v'}{\partial y})^2 + 2(\frac{\partial w'}{\partial z})^2 + (\frac{\partial v'}{\partial z} + \frac{\partial w'}{\partial y})^2 + (\frac{\partial u'}{\partial z} + \frac{\partial w'}{\partial x})^2 + (\frac{\partial u'}{\partial y} + \frac{\partial v'}{\partial x})^2 dV \quad [W]$$

$$E_{mean} = \frac{1}{V}\frac{1}{T_{CC}}\int_{CC}\rho\int_{V}\frac{1}{2}(u^2+v^2+w^2)dV dt \quad [\frac{J}{m^3}]$$

To gauge the pulmonary artery's performance η, normalization of energy losses (Elosses) is undertaken using the mean kinetic energy of each case studied (Emean) during the cardiac period (CC).

$$\eta = \frac{-E_{losses}}{E_{mean}} \quad [-]$$

Several critical fluid dynamics concepts are explored. Vorticity, which denotes the local rotation of a fluid, is utilized to understand flow patterns, and scalar quantities are formulated for each simulation. Helicity, showing the alignment between vorticity (previously calculated) and velocity fields (direct CFD result), offers insights into flow structures and their stability, with specific scalar metrics being developed for comparison.

$$H = \omega \cdot u$$

Lastly, the Q-criterion assists in identifying vortex structures in fluid flows, serving as a tool to visualize and comprehend the dynamics of cardiovascular flow. This criterion helps to understand intricate cardiovascular mechanisms and is often visualized using color mapping techniques.

4. Results and discussion

4.1. CFD analysis

Preliminary analysis

The study examined different cases with varying inlet conditions. The analysis focused on kinetic energy over time (fig. 3), with the acceleration phase occurring in the first 20% of the cardiac cycle, followed by the systolic peak between 20% and 25%. The analysis also considered the deceleration phase and a minor peak at 60%.

The kinetic energy curve correlated with volume flow at the inlet, indicating a direct proportionality. The study emphasized examining the systolic peak, acceleration, and deceleration phases at specific time points, respectively 15%, 23%, and 27% of the cardiac cycle. The peak of kinetic energy corresponded to the systolic peak, as confirmed by blood flow analysis at the inlet over time.

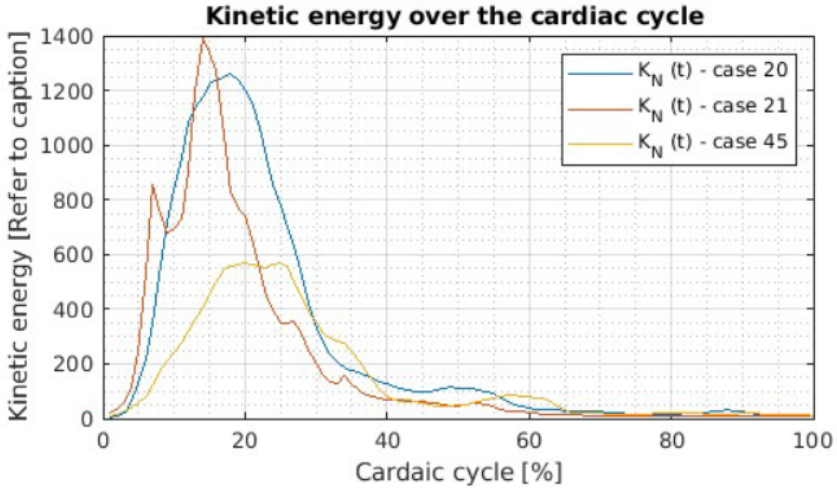

Figure 3 : Kinetic Energy over the cardiac cycle for three representative cases [pJ]

Vorticity, helicity, and Q criterion patterns exhibited similarities to kinetic energy during the cardiac cycle (fig. 4).

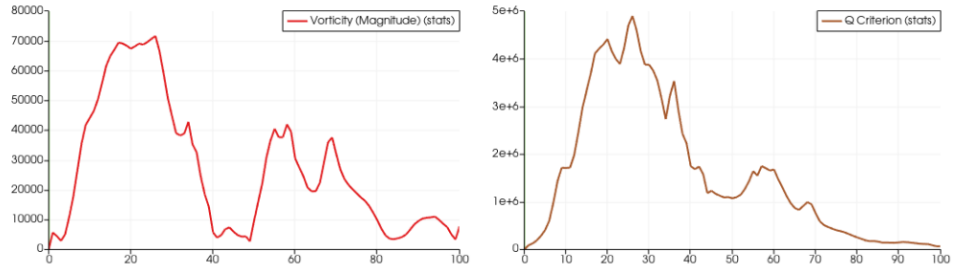

Figure 4 : Quantities integrated over the volume as function of time: vorticity on the left and Q-criterion on the right

Flow field

Velocity patterns in the main pulmonary artery (MPA) were analyzed during different phases of the cardiac cycle (fig. 5). During the acceleration phase, a relatively laminar flow with uniform distribution was observed across the MPA surface, and the inlet exhibited a weakly parabolic shape, with flow predominantly oriented toward the outer MPA wall. However, during the systolic peak, the flow ceased to be uniformly distributed, concentrating primarily on the outer wall of the MPA. Notably, a specific feature in the inlet conditions, marked by an isolated velocity peak on the inner wall of the MPA, was observed during the acceleration phase. This feature, not seen in some other cases, persisted throughout the acceleration phase, suggesting potential interactions between blood flow and upstream elements like the pulmonary valve.

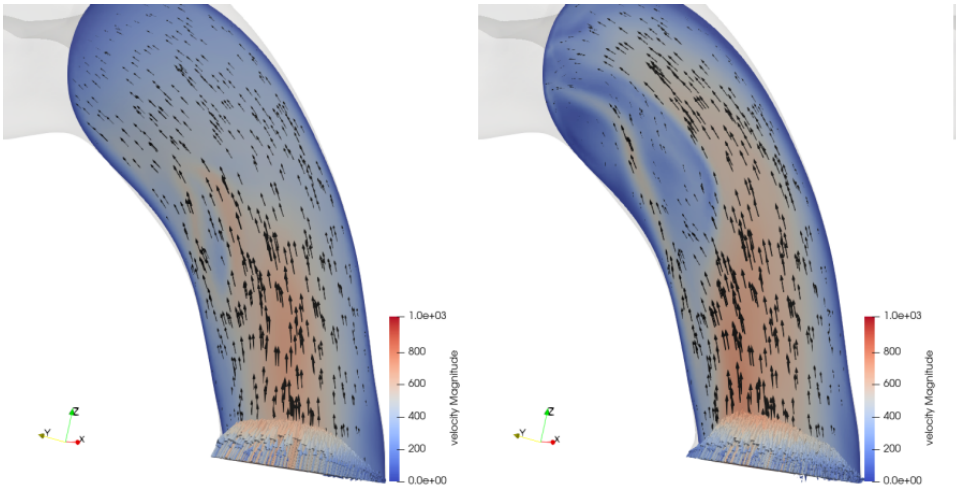

Figure 5 : MPA velocity with in-plane vectors and 3D inlet conditions during acceleration (left) and peak systole (right)

Pressure variations in the MPA were also examined (fig. 6). During acceleration, significant pressure was observed at the inlet, while a lower pressure was present at the right pulmonary artery/left pulmonary artery (RPA/LPA) split.

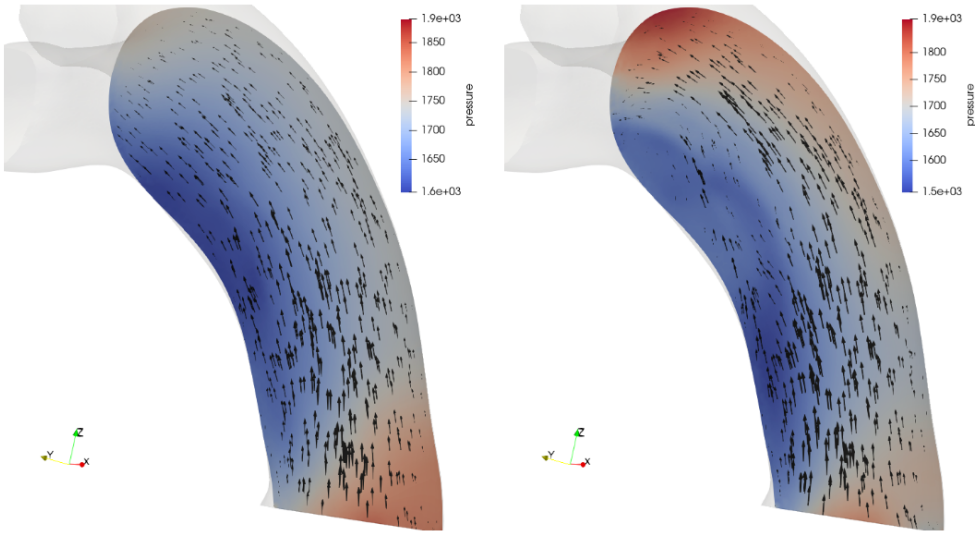

Figure 6 : MPA pressure with in-plane vectors and 3D inlet conditions during acceleration (left) and peak systole (right)

Additionally, a pressure differential existed between the outer and inner MPA walls, with a depression zone concentrated at the MPA's curvature. At the systolic peak, the pressure at the RPA/LPA split approached that of the inlet pressure, with a pressure peak at the split where blood flow was concentrated. During decelera-

tion, the pressure at the inlet became lower than at the split, leading to a significant pressure difference and partial flow redirection at the RPA/LPA split.

Helicity is a scalar quantity that measures the degree of alignment between the vorticity and velocity fields in a fluid. This alignment signifies how much the fluid flow swirls along its direction of motion. The analysis revealed the presence of a relatively constant helicity zone along the inner wall of the lower part of the MPA, which expanded over time upstream and downstream of the curvature region. During acceleration, a helicity peak was observed near the inner wall of the MPA, likely attributed to the curvature effect and interactions between blood flow and upstream elements like the pulmonary valve (fig. 7). The recirculation effect observed upstream of the curvature resulted from wall shear layer detachment on the MPA, with significantly higher helicity in this region compared to laminar flow regions [1]. Additionally, significant helicity was observed in the lower part of the RPA/LPA split, where flow redirection toward the inner wall led to vortex-like patterns.

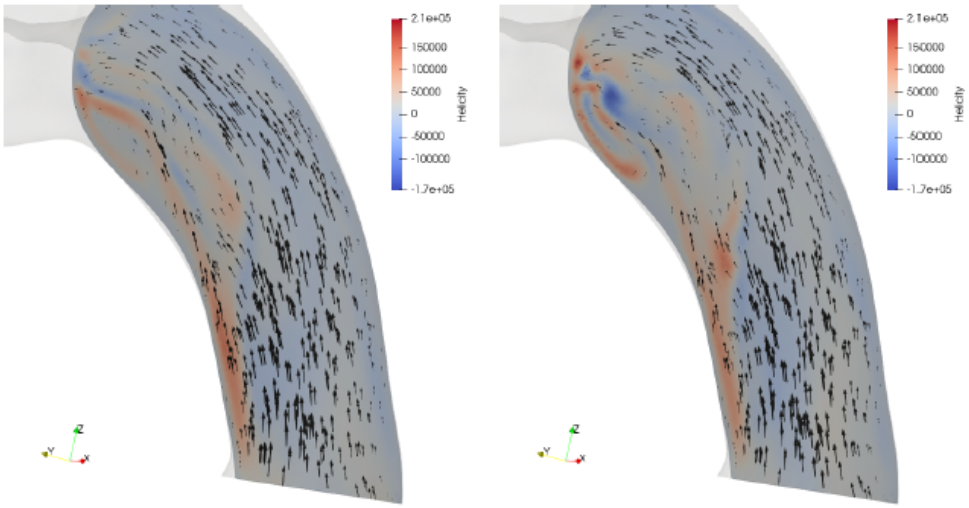

Figure 7: MPA helicity with in-plane vectors and 3D inlet conditions during acceleration (left) and peak systole (right)

Vortical structures

The examination of the MPA revealed a primary vortical structure originating upstream of the MPA inlet, coinciding with the structure observed during the acceleration phase. This primary structure was situated on the inner side of the MPA.
Additionally, a second vortical structure was identified, originating from initial conditions at a different temporal moment and located between the inner and outer parts of the MPA (fig. 8).

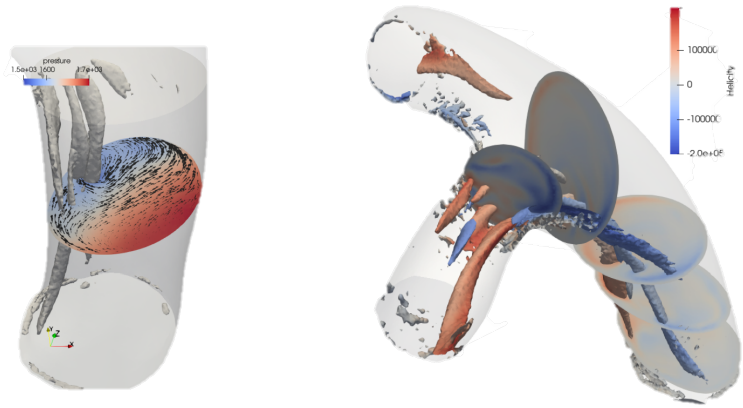

Figure 8 : Formation of vortical structures during systole peak highlighted using Q-criterion isosurfaces

Another distinct structure developed on the inner MPA wall as the curvature increased (fig. 9). Unlike the initial conditions, this structure was associated with the curvature itself and was influenced by the transverse pressure gradient, inducing motion and circulation along the MPA walls, ultimately forming a swirling zone.

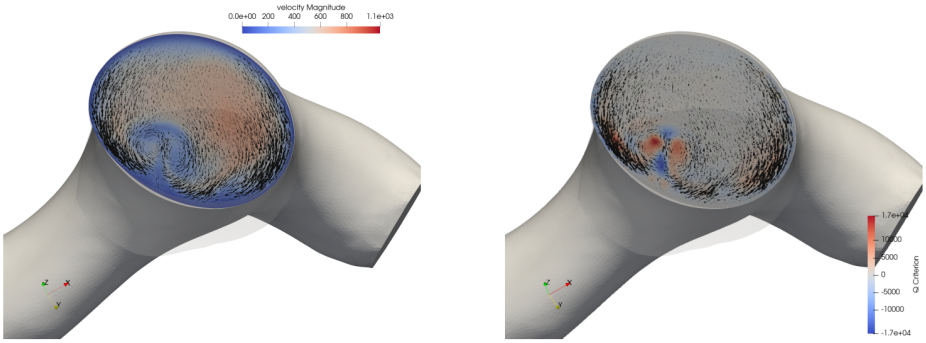

Figure 9 : Slice of the MPA with in-plane velocity vectors - Dean vortices in the vicinity of the inner wall due to curvature

The curvature of both the right pulmonary artery (RPA) and MPA was found to generate secondary motions. Vortical structures observed in the MPA extended into the RPA (fig. 10) [9]. Notably, the helicity reached significant levels at the curvature of the RPA. In contrast, the left pulmonary artery (LPA) exhibited fewer vortical structures due to its relatively straight geometry. The curvature-induced secondary motion was evident in visualizations, with the RPA's curvature creating a low-pressure zone on its inner wall, leading to the generation of vorticity in those regions. This vortical structure formed at the bifurcation and stabilized within the RPA. Vortices were also observed near the inner wall of curvatures in both the

MPA and RPA, resulting from the interaction of velocity peaks and low-pressure areas induced by curvature. This phenomenon was identified as Dean vortices in scientific literature [10].

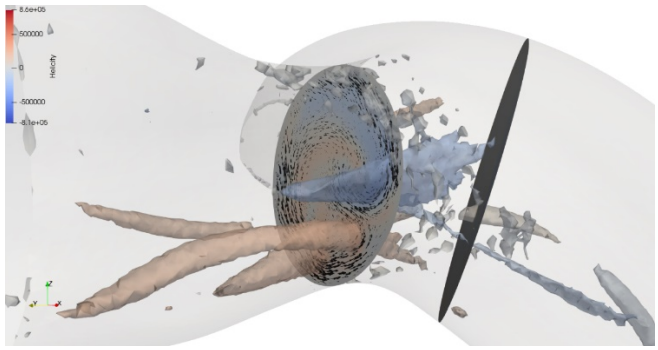

Figure 10 : Vortical structure observed in the RPA during peak systole, emphasized using Q-criterion isosurfaces

During the deceleration phase, a different type of swirling motion was observed, originating from the MPA's bifurcation and extending into both the RPA and left pulmonary artery (LPA) (fig. 11). This phenomenon was attributed to wall shear layer detachment triggered by the MPA's curvature, which induced a positive pressure gradient [1, 11].
The velocity field caused the elongation of the vortical structure as the flow divided into the two branches. Additionally, flow orientation from the outer wall to the inner wall occurred when the MPA flow met the RPA/LPA split, a phenomenon previously documented by Bachler et al [3].

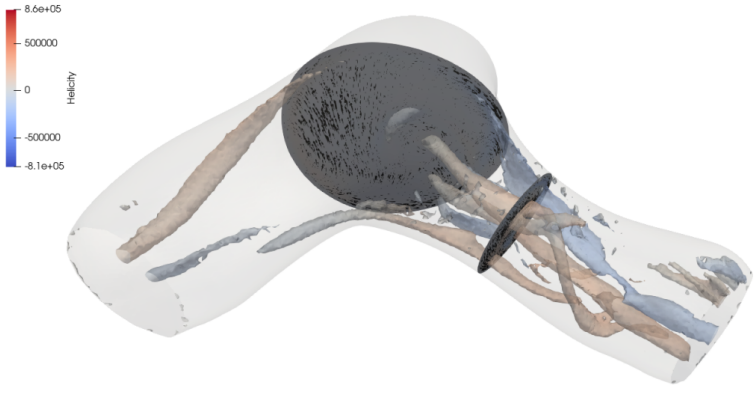

Figure 11 : Vortical structure formation between the RPA and LPA (deceleration)

4.2. Global characterization results

Correlations in between different quantities

Average kinetic energy in the pulmonary artery (PA) reflects conditions at the inlet, but there is significant variability in initial conditions. A statistical analysis revealed direct proportionality between average kinetic energy and numerous other quantities. Two quantities, η (PA performance) and volume, do not appear to be correlated with the mean kinetic energy (Emean) over a cardiac cycle. As seen in the previous chapter, η is the ratio of energy losses to mean kinetic energy, and it doesn't exhibit proportionality due to varying divisor values. Volume of the PA (V) has lower variance, allowing correlations to be maintained when normalizing values by volume.

R [10^2]	Emean
Emean	-
Elosses	95.99
η	-1.74
H	92.53
ω	50.09
V	-6.72

Generalizing results is challenging due to variability in inlet conditions, a limitation of the study. Quantities correlated with volume are η and Helicity, and a correlation between Elosses and Emean has been highlighted. The definition of η and the discovered correlations imply a link between Elosses and quantities influenced by initial conditions, such as volume and Emean. Therefore, η may be correlated with multiple quantities like the inlet conditions or the volume of the PA, independently of the normalization. Verifying this hypothesis would require the development of a new methodology allowing to reduce initial conditions variables between each case studied. This would allow to have more comparable results instead of having shape and inlet conditions varying at the same time. One way of exploring this would be to use SSA in order to develop an averaged inlet condition over the various cases, which could be then adapted to the shape of the inlet.

Correlations in between quantities and modes

The SSA analysis identify parameter with a specific impact on the geometry. However, variation in a mode (mathematical parameter characterizing the shape of the PA based on a reference shape) often affects multiple parameters, making it challenging to utilize the modes to establish a direct link between a specific geometric characteristic and a physical quantity. Despite this difficulty in associating modes with geometric variation, it might be interesting to make the following assumption about modes, increasing:

- mode 0 increases the volume
- mode 2 reduces the angle between the RPA and the MPA
- mode 3 reduces the curvature of the MPA

• mode 4 reduces the overall vessel size (and consequently the volume)

A correlation between M0 and PA volume is observed, like the correlation observed with other quantities associated with volume. M3 shows correlations with various quantities, but it doesn't appear to be correlated with volume, unlike η and Helicity. The correlations observed are statistically significant. A hypothesis suggests that an increase in M3 leads to a reduction in the curvature of the main pulmonary artery (MPA), which could potentially reduce vortical structures and improve PA performance.

R [10^2]	V	M0	M1	M2	M3
Emean	-6,72	1,0	1,7	10,2	-57,5
Elosses	-25,3	-9,7	12,3	11,1	-57,0
η	-61,2	-39,8	27,4	13,7	-6,8
H	-18,6	-5,7	12,5	8,4	-57,7
V	-	66,9	-36,3	-10,3	5,0

The analysis assumes linear correlations, but the data might have different, possibly higher-order correlations. Polynomial regression analysis is suggested as a method to identify higher-order relationships between variables, but it requires the development of statistical indicators. The current information doesn't allow for conclusive findings, and further analysis and investigation are needed to understand the relationship between curvature reduction and PA performance, especially in terms of potential higher-order correlations.
The models studied in this research encompass a combination of all these factors in varying proportions. Consequently, this complexity is likely to make the comparison process of a single mode at a time more challenging.

5. Conclusion

The research project aims to advance our understanding of the flow field in the pulmonary artery, an area that is relatively understudied due to its complexity. Therefore, the study contributes to the knowledge gap in pulmonary artery flow and has the potential to improve clinical management of pulmonary vascular diseases.

The project combines computational fluid dynamics (CFD) simulations with in-vivo data to analyse flow patterns and their underlying mechanisms. Advanced tools and methodologies, such as statistical shape analysis and scalar quantities development, are used to explore correlations between different variables and parameters. The development of specialized scripts and tools enhances data pro-

cessing and analysis. Rigorous approaches, including anomaly identification and filtering techniques, ensure the reliability and validity of the results.
Limitations include variability in in-vivo inlet conditions, modelling assumptions, and the need to strike a balance between realistic conditions and generalizability. Designing inlet conditions resembling real-world scenarios is crucial for meaningful comparisons. Non-in-vivo data can provide a common basis for comparison but requires careful consideration of the inlet plane's orientation. Automation and refinement of simulation and data processing techniques will enhance accessibility and efficiency. Finally, future investigations may focus on the physiological implications of observed vortical structures and early diagnosis biomarkers for pathologies.

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