Computational Fluid Dynamics (CFD) study of patients suffering Coarctation of the Aorta (CoA) for pre and post-operative

BY

Omar Osama

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering

Under the supervision of:

Mohamed El-Morsi
Associate Professor, Department of Mechanical Engineering

Khalil El-Khodary
Assistant Professor, department of Mechanical Engineering

The American University in Cairo

May, 2017
To my Family, Friends and Marlene Mumper.
Acknowledgements

I would like to express my thanks for all who helped in making this study possible. My supervisors Dr. Elmorsi and Dr. Elkhodary, for their scientific support and guidance. Dr. Ing. Heba Aguib and Magdi Yacoub Foundation (MYF), for their support in the medical area and providence of the data of the patients. Dr. Ryo Torii for sending the MatLab and FORTRAN codes used for mapping the boundary conditions from the PC-MRI. Engr. Amr Sami, Engr. Mohamed Osman, Engr. Mohamed Atef, Engr. Hani Mashaal and other people working in OPTUMATICS, for their technical advises.

Omar Osama
May 2017
Coarctation of the aorta (CoA) is a widespread anomaly that occurs a lot in infants. CoA affects human health. It causes hypertension, decrease in the amount of blood flow and heart failure. CoA is related to abnormal hemodynamics and certain blood flow patterns are noticed. Different surgical techniques are implemented in order to increase the amount of blood flow such as resection end-to-end anastomosis, resection end-to-side anastomosis…etc. This research aims at identifying the effect of CoA on the flow pattern and quantification of the improvement after surgery through utilizing computational fluid dynamics (CFD) to solve flow fields in the aorta.

CFD is applied on a real geometry of the aorta are obtained by computerized tomography (CT) scan for five pre and post-operative patients. The boundary conditions are derived from phase contrast magnetic resonance imaging (PC-MRI). Then, grid independence and time sensitivity analysis are performed. Flow patterns are judged visually by comparing the contours of the streamlines, vortex core, pressure and the time averaged wall shear stress (TAWSS).

In order to quantify the flow fields and the improvement as well, different flow variables are used such as Womersley number, Strouhal number and specific turbulent kinetic energy. The wall shear stress at peak systole and the amount of the blood flow in the direction of the vessel's centerline are used as a measure of improvement.

The results of the CFD showed that blood flow patterns are highly dependent on the geometry of the vessel. For a CoA, jet formulation then break up, backflow and chaotic behavior exists after the area of the disease. In addition, a high concentrated wall shear stress is around the area of the
CoA. For post-op, the change of the area because of the surgery produced separation. For both pre- and post-op, the angle between the velocity vector at the inlet and the centerline of the vessel resulted in a jet impingement and very high wall shear stress. On the other hand, the specific turbulence kinetic energy and the wall shear stress is higher after the surgery. Strouhal number in the descending aorta has decreased after the operation except for one patient. The amount of blood flow increased after the surgery. Blood flow in the downstream became attached to the vessel. Finally, the flow fields are sensitive to the turbulence model; however, they did not show significant dependence on the viscosity model. The turbulence effects cannot be neglected due to their significant contribution to the velocity field.
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1. Introduction

The cardiac muscle (heart) is responsible for transporting and circulating the blood flow through the arteries and veins to the organs of our body. It can be modelled as an electro-mechanical pump.

The role of arteries, with the exception of the pulmonary artery, is to carry the oxygenated (fresh) blood in order to be used by other organs. Veins take the used blood (deoxygenated) back to the heart.

Aorta is the largest artery in the human body. The heart contains four chambers; right atrium, left atrium, right ventricle and left ventricle. They are connected to each other and to the other arteries through different valves. The valves between atria and ventricles are called atrioventricular valves (mitral and tricuspid valve). The valves between the ventricles and arteries are called semilunar valves (aortic and pulmonary).

1.1 Cardiac Cycle

The cardiac cycle is divided into five main portions. Wigger’s diagram is a diagram that shows the changes of pressure, volume, electricity, and heart sounds through the cardiac cycle. Such sounds arise from opening and closure of valves. Table (1.1) summarizes the different processes in the cardiac cycle.

\[1\]
Phase 1 Atrial Depolarization
Right and left atrium are contracting.

Phase 2 Isovolumetric Contraction
This phase lasts for very short time. When AV close beside SV did not open yet (all four valves are closed) so the volume of the ventricle is constant.

Phase 3 Ventricular Ejection
Ventricular pressure rises above the aortic and pulmonary arteries pressure causing their valves to open resulting in ejection of blood to our organs.

Phase 4 Isovolumetric Relaxation
Again, SV close so all of four valves are closed because of pressure of ventricle became less than aortic pressure.

Phase 5 Ventricular Filling
When the ventricle pressure is below atrium pressure the AV open again repeating the cycle.

Table 1. Summary of the Cardiac Cycle
1.1 - Aorta
It is the largest artery in our body going out of left ventricle. It is connect to the left ventricle by means of aortic valve. Healthy aortic valve is tricuspid. Aortic valve is responsible for controlling the blood flow gushing out of ventricles into aorta, by means of the difference in pressure between the left ventricle (upstream) and the aorta (downstream). Aorta contains different regions: aortic root, ascending aorta, aortic arch and descending aorta. Three branches go out of aorta in order to transport the blood to the upper body. The left common carotid artery sends blood from aortic arch to the neck. The left subclavian artery sends the blood to the left arm. The brachiocephalic artery is divided into two arteries: the right common carotid and right subclavian artery. Similarly, the...
The right common carotid sends the blood to the neck and the right subclavian artery transports the blood flow to the right arm. The blood continues flowing down the lower body across descending aorta. Figure (1.1) shows the shape of aorta and its various regions.

**Figure 1.1: Anatomy of the Aorta**

The wall of aorta consists of three layers: endocardium (most inner), myocardium (middle layer) and epicardium (most outer). They differ in the structure and the function as well. The inner layer is very smooth in order to keep the blood flows without causing clots or disturbances. The role of the middle layer is to withstand the mechanical stresses. The outer layer is a thin one for protection. Figure (1.4) shows the different layers of the wall of aorta.

- **Aortic Root**
- **Ascending aorta**
- **Brachiocephalic artery**
- **Left common carotid artery**
- **Left subclavian artery**
- **Descending aorta**
Development and Anomalies in human aorta

The process of development of aorta may occur in wrong way leading to different anomalies.

1. Anomalies with left Aorta.
   The right subclavian artery is raising behind the esophagus in an abnormal manner (retro-esophageal). It presses on the trachea and results in dysphagia lusoria. When the right ductus arteriosus does not close after the birth, it makes a virtual vascular ring. In this case, the aortic pressure is increased and hence the blood flow goes back from aorta to the lungs again, which decreases the amount of blood flow going to the aorta. Figure (1.2) shows a computerized tomography (CT) angiography scan for a 5 years old patient with aberrant retro-esophageal right subclavian artery.

2. Anomalies with right aorta
   This anomaly changes the order of the arteries raising out of the aorta. The most common anomaly in this category is right aortic arch with mirror image branching. The right arteries come after the brachiocephalic artery, which is branching into left carotid and left subclavian arteries.
Figure 1.3 Mirror imaged branching anomaly

Anomalies with double aortic arch

The thoracic aorta is divided into two aortic arches that encircle the trachea as shown in Figure (1.4).

Figure 1.4 Double sided anomaly in aorta,

Coarctation of the Aorta (CoA)

CoA is defined to be a narrow area that usually appears after the left subclavian artery as shown in figure (1.5). It causes a high pressure in the upper body (hypertension) and low pressure in the legs or lower limb. Narrow area can be modelled as a resistance so heart load increases to pump blood through narrow area. CoA affects also the fluid mechanics of blood through the aorta in terms of pressure, velocity and flow regime. Because of the abrupt...
change in area, vortices and turbulence occur just after the Coarctation.

Figure 1.5 Coarctation of the aorta

Bicuspid aortic valve (BAV)

The aortic valve usually contains three cusps. However, in some cases it is formed only by two cusps and called bicuspid aortic valve (BAV). BAV happens in 1-2% of population and results in higher velocity and stresses on the walls of aorta.

1.3 CFD for Bio Fluids

Although the advances in imaging techniques, the spatial and temporal resolutions are limited. It cannot provide the values of flow fields neither in the whole organ nor for many time slices. Moreover, the limited spatial resolution results in not being able to estimate true values of wall shear stress because the boundary layer thickness is much smaller than the size of the voxel. On the other hand, CFD does not only help in estimating the forces and stress on the walls. It can be used to calculate the amount of low density lipoprotein (LDL). CFD is essential for virtual surgeries as well, and can be used in designing different stents or trying different surgeries numerically in order to find the best solution for a specific patient or a certain group of patients.
Bibliography


2. Literature Review

Numerical simulations can work as a barrage to deep understanding to different problems that are expensive to be analyzed experimentally or there is no experiment to be conducted at all such as in medical surgeries beside giving a wide stream of information at every point in the domain.

Engineering can help in analyzing and understanding how our body works since we have chemical reactions, mass transfer, fluid mechanics, stresses and deformation, and electro physiological phenomena. In the cardiovascular field, Engineering approaches have been developing imaging techniques to analyze the cardiovascular system components such as ventricles, aorta... etc. Using PC-MRI, it is possible now to extract the dimensions and velocity fields, and turbulence. Whereas 4D flow techniques can show the stream lines as well. Despite the advance in imaging techniques, resolution is not sufficient to give information about different quantities such as wall shear stress, mass transport...etc. That is why numerical simulations in general will help in understanding healthy cardiac function as opposed to abnormal cases. Recent research has been conducted on different biological problems such as an electro-physiology analysis of the ventricle, the flow field in the aorta, bio-mechanics of our bones, nano-technology and its role in fighting cancer... etc.

The physics of cardiovascular flows can be very complex to simulate; blood is a non-Newtonian fluid, the walls are viscoelastic, boundary conditions are time varying and difficult to select. That is why the fluid problem of blood flow in the arteries can be solved in wide spectrum of complexity. However, the goal of the simulation determines the complexity of the solution and the possible assumptions or physics that can be ignored without having a significant effect on the pressure and velocity fields.
A change of area has a significant effect on hemodynamics in cardiovascular flow since stenosis in general comes with turbulence and can adversely affect the heart's work. Idealized pipes with different severity or change in area have been studied experimentally and numerically in order to find the best method to simulate this kind of problems besides understanding the origins of turbulence. The solutions to turbulence range between zero equations (the cheapest method) to DNS (the most expensive) with several levels of modeling in between. The level of modeling is related to the level of information that we are interested in knowing. If the goal of simulation is to compare between the hemodynamics of different arches, then maybe a two equations model is enough. However, if the question is how the turbulence behaves or how its eddies are structured then the simulation should be done through either LES or DNS.

The following literature review summarizes several points: nature of pulsatile flow, flow in bends, blood flow in healthy aorta, effect of valve morphology, stenosis and Coarctation of aorta, boundary conditions and different models of blood viscosity.

2.1 - Pulsatile flows through bend Anthanasia Kalpakli [1] reviewed the different structures of flow downstream bends in steady and pulsatile cases, conclusions of different experiments, the numerical simulations and the used models and the important numbers to describe pulsatile flows. It is important to understand the pulsatile flow because the heart pumps blood in a similar manner and the aorta has a beneficial shape. There are five different patterns of downstream pulsatile flow through bends, which are:

a. Dean circulation.
b. Deformable Dean Circulation.
c. Intermediate circulation between Dean and Lyne.
Defor-mable Lyne circulation.

Lyne Circulation.

Figure 2. Vortices downstream bend

A low Reynolds number is associated with dean vortex type and a high Reynolds number produces Lyne type. In this experiment, the range of Reynolds between 50 and 450 and the Womersley number was between 7.5 and 25.

Daniel Feldmann et al. [2] used DNS simulations to solve pulsatile flow in straight pipe. His findings show how combination of inlet parameters can affect flow field regime making it laminar, turbulent or transitional. However, since it is not sufficient to use the Reynolds number to categorize pulsatile flow, a Womersley number must be taken into account. This has been proven numerically and experimentally. Feldmann’s three DNS simulations confirmed the experimental conclusions. The first DNS simulation was performed at Re=2890 and Wo=26 and the pulsatile flow was laminar without any noticeable instabilities. For the second case, Re=11460 and Wo=13, low was conditionally...
unstable in the deceleration phase then became laminar again in acceleration. The axial velocity and transported to radial and azimuthal components generated turbulence in the second case. Finally, the pulsatile flow was fully turbulent at \( Re=22540 \) and \( \omega_0=5 \).

2.2 - Hemodynamics in Healthy Aorta

For a normal healthy aorta, blood flows in the direction of the arch wall during acceleration (early systole) with velocity skewness towards the inner wall. Reaching mid systole, the peak velocity moves outward, helical structure starts to appear and separation occurs. This differs according to arch geometry; the shape of the ascending aorta, which may be twisted or flat; and the angle of curvature of the thoracic descending aorta.

Blood flow in human cardiovascular system is laminar in general while it is transitional in large arteries such as aorta. Kousera et al. have performed a numerical study to discover how the instability inside aorta occur by changing the inlet mass flow rate wave on the same aorta using transitional to turbulent model which is capable to capture transition from laminar to turbulence concluding that aortic flow with low Reynolds and Womersley numbers can be modeled as laminar. Stalder et al. worked on defining ranges of Reynolds number that can be used to classify flow into laminar or turbulent. In his PC-MRI study, eight planes had been taken for thirty young healthy volunteer to correlate the critical Reynolds number with Womersley and Strouhal numbers. It could be noticed beside the correlation that turbulence or transition from laminar to turbulence is more probable while increasing body weight, cardiac output and in males more than females.

\[ R_e^p = 169 \alpha_0^{0.83} \sqrt{S_t - 0.27^2} \]
Inlet Boundary Condition

John F. LaDisa et al. [6], [7], performed several numerical simulations on different arches in order to determine the effect of the aortic valve in simulations. Using two different types of inlet boundary condition: mass flow rate and realistic velocity profile obtained from PC-MRI and applying three-element windkessel model at outlet boundaries, and modeling blood flow assuming turbulent flow regime.

Windkessel model is a lumped electrical analogy that predicts the pressure in the aorta as shown in figure 2.2. It reduces the system into an electrical circuit, which has resistance and capacitance. As a result, inlet boundary condition affects local indices of time-averaged wall shear stress and turbulent kinetic energy since mass flow rate or a plugged in velocity at inlet underestimates turbulence. That is why realistic boundary condition at inlet of aorta should be used. Besides comparing different cases (normal, native CoA, arch treated by end-to-end, and arch treated by stenting) showing that CFD is useful in predicting areas that suffer from high shear stresses or abnormalities due to surgeries.

Figure 2.2 Two Elements Windkessel Model

Matthias Baeur et al. [8], analyzed 58 persons with valve stenosis (BAV or TAV) echocardiographically showing that in case of BAV a higher peak velocity in anterolateral region in ascending aorta compared to TAV.
Model Problem of Stenosis (CFD Model) 

J. Ryval et al. [9], used a two equations model. In this study, standard and transitional K-ω models have been used to solve ideal pipe with 75% stenosis and comparing velocities and turbulence with those obtained experimentally by Ahmed and Giddens. Transitional turbulence model K-ω is more suitable in this case because it has the ability to correct itself and back to its laminar situation again. Standard K-ω model is over estimating turbulence in this case.

Another popular two equations model is k-ε model with its three types, low Reynolds number, RNG, and standard K-ε. Simulating the same problem of Ahmed and Giddens as well showed that standard K-ω qualitatively and quantatively estimating velocity compared to K-ε. [10]

DNS has very accurate representation of fluid problems because it solves all of time and spatial scales with no models or approximation but it is not suitable for commercial uses. It is for research uses only. On the other hand, LES can resolve eddies that contain the high energy and model the rest. LES is expensive with respect to standard RANS family but more accurate than them. The velocities obtained from LES showed great match with DNS and LDV measurements [11].

Two cases have been simulated for steady state and pulsatile flow at inlet using DNS simulation by Steven Frankel and Sonu S. Vargeshe [12], [13]. There are two geometries included in this study one with eccentric stenosis and the other with axisymmetric one. In case of steady state, Laminar flow regime existed at low Reynolds number (Re=50) while increasing Reynolds number (Re=1000) caused turbulence after stenosis in case of eccentric geometry only. While, for pulsatile wave at inlet, reverse flow starts to appear post stenotic near mid acceleration with localized turbulent region between 2 and 3 times diameter of the pipe downstream the stenosis. Flow reattaches again after 7 times the diameter of the pipe and became laminar again around 11.
times the diameter for eccentric geometry. For axisymmetric geometry, distance of recirculation and transition to turbulence is larger.

2.5 - CFD in Aorta

Amirhossein Arzani et al. [14], applied DNS on aorta to compare turbulent kinetic energy between simulation and from PC-MRI reaching maximum relative difference between DNS and estimated turbulent kinetic energy (TKE) was in order of 10%. A very important note is that the max. TKE appeared just after peak systole. In general, there was agreement between the experimental and numerical turbulent kinetic energy.

J.Lantz et al. [15], compared the turbulent kinetic energy numerically using LES and experimentally using PC-MRI between pre and post-operative aorta who was suffering Coarctation treated by balloon dilation. Blood is laminar in accelerating phase confirming that turbulence start to occur near peak flow. Moreover, fluctuations do not start at Coarctation only but earlier to it near branching vessels. Another important note is that the maximum turbulence was at mid deceleration. Intervention of Coarctation reduced the total kinetic energy overall the arch but it did not disappear.

Lauri J Oliveri et al. [16], investigated the location of maximum wall shear stress on aortic wall. Post-operative aortic wall shape can be classified into Crenel, Gothic, and Romanesque. The researcher used turbulent K-\(\Omega\) at peak velocity to find the difference in wall shear patterns on the three repaired arches. The main finding is that Peak WSS is located in the isthmus of the Gothic model and the variations between normal and repaired arches comes from abnormal modeling of the wall which may have effect on vascular dysfunction.

John F.LaDisa et al. [17], presented the simulation of five arches in different conditions (normal, native moderate CoA, native severe CoA, CoA patient treated by end to end,
and CoA patient treated by end to end (side) solving continuity, Navier Stokes and wall motion equations. Volumetric flow rate at inlet and windkessel model at outlets have been used as boundary conditions. The conclusion of this work in brief is that CFD can be a decision tool in some cases by quantifying if the cardiac performance is acceptable or not, rotation in TAWSS and OSI was noticed as well which might suggest formation of plaque in different areas. In different study, solving only continuity and Navier-Stokes equations, comparing only CoA patients treated by end to end with control cases, it was shown that the overall TAWSS did not differ much between the two groups while a left-handed rotated pattern in local TAWSS has been noticed as well.

J. Lantz et al. [18], studied the effect of the age on the wall shear stress in aorta. Two groups have been studied (8 persons in the old group and 10 in the young one) using laminar Newtonian fluid model. TAWSS significantly differed between two groups (p-value is 0.05) while OSI did not differ much. He also continued his work and quantified turbulent wall shear stress in aorta using LES to resolve the turbulence in aorta. In addition, he worked on simulating fluid structure interaction using fully coupled solver for the problem of a healthy aorta using shear stress transport for fluid model and solving stresses and deformation for different Young’s modulus since there is no global one for arch solid wall, which was modeled as linearly elastic material. A simple elastic support has been used as a boundary condition to simulate the effect of damping of other organs around aorta. As a result, FSI changed the pattern of both instantaneous WSS while the TAWSS and OSI changed slightly [19]. Another resolved physical phenomena in heart is LDL transport and accumulation on the wall of aorta [20]. The modeling of concentration of LDL is according to the following transport equation:

\[ \frac{\partial C_w}{\partial t} + \mathbf{V}_w \cdot \nabla C_w - D \frac{\partial C_w}{\partial n} |_{w} = K_w C_w (2) \]
The flow field was resolved using Large Eddy Simulation. The results showed adverse relation between the concentration of wall shear stress and concentration of LDL. Moreover, LDL has more concentration during systolic declaration and vice versa.

Zahra Keshavaraz et al [21], in her study of three cases, Healthy aorta with normal tricuspid aortic valve (TAV), aorta with Coarctation with TAV, and aorta with Coarctation with bicuspid aortic valve (BAV) at the inlet are modeled. A laminar simulation was performed for the first (healthy) one while a transitional k-ω model was used for the arches with Coarctation. The boundary conditions were flat velocity waveform at the inlet and outflow at the outlets. A validation was done using PC-MRI comparing velocity profiles obtained from simulations with measured velocities showing good matching. As a result, BAV increases velocity downstream Coarctation besides increasing TAWSS and OSI as well which means that BAV amplifies the abnormal hemodynamics due to Coarctation.

Z.Cheng et al. [22], used transitional shear stress transport model to simulate the problem of dissection of aorta using volumetric flow rate and zero pressure at outlets. CFD Simulation showed matching in velocity profile and flow rate in false lumen and with PC-MRI.
Modeling of Blood Rheology

Alistair G.Brown et al.

in his work investigated the question of accuracy and efficiency of simulation by solving the flow fields in two cases. First cylinder and the second case is arch according to three levels of complexity: fluid structure interaction (FSI), Compressible fluid model, and Incompressible fluid model. The used boundary condition is mass flow rate at inlet and windkessel pressure at the outlets. The results showed that compressible fluid model could be used to capture travelling waves in aorta while it is less complex than the fluid structure interaction one.

Safora Karim i et al. performed several simulations to figure out the effect of rheology of blood on hemodynamics inside aorta. The used boundary conditions are varying velocity at inlet and outflow at outlets. Nine non-Newtonian viscosity models have been used of three main categories: Casson type, Carreau type, and Power-law type. The global non-Newtonian importance factor was defined:

$$I_G = \frac{1}{N} \sum_{i=1}^{N} (\mu - \mu_\infty)^2$$

Where $I_G$ represents the grid index and $N$ is the total number of grid points (on the wall).

In addition, non-Newtonian effect factor $(NNEF)$ is defined as following:

$$NNEF = \frac{(\frac{\mu}{\mu_\infty})_{non-Newtonian} - (\frac{\mu}{\mu_\infty})_{Newtonian}}{(\frac{\mu}{\mu_\infty})_{Newtonian}}$$

The results showed that non-Newtonian effects appear more significantly in the low regime of velocities (diastolic phase). In addition, Cross models have the highest importance factor while Casson model have the lowest importance factor.
Outlets Boundary Conditions

Vignon-Clementel et al. [25], applied the model (Electrical analogy developed by Manetro) to account for the flow boundary conditions at the coronary arteries beside inlet of aorta while solving the flow field and wall motion using finite element.

Mahdi Esmaily et al. [26], compared between three methods to prevent divergence in simulations because of backflow by adding stabilization term, force velocity to be normal to the outlet, or using lagrangian multipliers. This study showed that stabilization method was better compared to lagrangian multipliers because of being less expensive computationally, easy, and more robust.
2.8 - Summary of literature review

Study Boundary Conditions Computational Domain Problem Statement/Conclusion

Numerical prediction of instability in aorta.

- Inlet: Volumetric Flow rate
- Outlets: Outflow boundary condition.
- 1.5% turbulence intensity at inlet.
- Mesh size: 1.2 M hexahedral elements.
- Outlets have been extended five lumen diameter to minimize effect of outflow boundary condition.
- $K-\omega$ SST transitional finding range for which blood flow in aorta is expected to be unstable.

Experimental Study on flow instabilities in aorta - Find empirical correlation between Strouhal number, Womersley number, and critical Reynolds number.
Numerical Study about inlet boundary condition in aorta

- **Inlet:** Volumetric flow rate and realistic flow at inlet from PC-MRI.
- **Outlets:** three-element windkessel.
- **Mesh size:** >3 M tetrahedral elements.
- Solution was obtained stabilized finite element method with LesLib commercial solver.

- Plugged in velocity under estimates TKE in aorta.
- BAV and TAV differentially affect distribution of TAWSS and OSI on aorta.

- Numerical study on two equations model in tubes with stenosis.
  - User defined velocity profile at inlet.
  - Mesh size: 139 K and 290 K hexahedral elements.
  - Standard and transitional shear stress transport model (k-ω).

- Transitional k-ω model is better for pulsatile flows because it corrects itself (has the ability to relaminize the flow again).

- Numerical study on two equations model in tubes with stenosis
  - Periodic velocity at inlet.
  - Mesh size: 30, 60, and 90 elements were on the radial direction for grid independence study.
  - k-ω and k-ε.

- k-ω model was much better in agreement with experimental data compared to k-ε in general.
Numerical study on tubes with stenosis

- Inlet: normal mass flow rate.
- Inlet: turbulence intensity was calculated using a variant of the vortex method.
- Mesh size: 6M.
- LES is the most accurate model to capture transitional flows in pipes with stenosis.

Turbulence estimation in Aorta

- Inlet: plug profile that matches with experiments.
- Outlets: 3 elements windkessel model with lagrangian method.
- Tetrahedral mesh with maximum edge size of 250 micron at the descending aorta.

DNS PC-MRI and DNS agreed qualitatively in capturing turbulence intensity with maximum error of 10%.
Turbulence assessment in Aorta.

Inlet: measured from PC-MRI. Outlet: pressure boundary at descending aorta.

- Mesh size: 7M anisotropic hexahedral.
- LES Turbulence still exist near the location of Coarctation or treatment.

WSS in repaired Aorta

- Mesh size: from 126 to 577K hexa core elements.
- $k-\omega$ Treated aorta exhibits higher peak WSS than normal beside Gothic arch showed high shear stress in specific location downstream.

Hemodynamics in repaired aorta by RWEA (6 treated and 6 control)

Inlet: mapped waveform. Outlet: Three elements windkessel

- Mesh size: 3 M tetrahedral
- Laminar FE solver

Distribution of TAWSS and OSI differs between treated and control cases.
Representative sample of Aortic patients (Pre and Post) Inlet: wave form Outlet: Three elements windkessel.

- Mesh size: 2-3 M
- Laminar incompressible equations for the fluid and the elasticity for the solid wall.

Comparing TAWSS, OSI, and deformation at different regions in aorta for normal, moderate CoA, severe CoA, CoA treated by end to end, and CoA treated by end to side at rest and exercise.

Rheological effects of blood Inlet: velocity profile Outlets: mass flow rates

- Mesh size: 1.7M with hybrid elements
- Laminar Cross non-Newtonian models produce higher effect of rheology of blood compared to Casson.

Flow in coronary arteries Closed loop model with an inflow boundary condition coupled with the simulation

- Mesh size: 1.7M for normal case and 1.8M for coronary with 40% stenosis.
- Continuity, Navier-Stokes equation and elasticity equations using Finite Element.

Solving flow fields and deformation in coronary arteries only by applying closed loop model at boundaries.

Table 2

1 Summary of the literature review


Mathematical Modeling


The conservation laws are the pillars of physics and by using them, we can derive a set of equations that describe the flow nature. An important assumption is that fluid is continuum. The idea of continuum is to assume that we can deal with an infinitesimal element of fluid rather than going deeper to atomic structure. An infinitesimal is much bigger compared to the structure of atom but still much smaller compared with the scales of material kinematics. The barrier between molecular and continuum scales is defined to be Knudsen number.

\[ \frac{1}{Kn} \leq \lambda \]

For a continuum approach

\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho U) = 0
\]

3.1.1 The Conservation laws

1. Conservation of mass. "Mass can neither be created nor destroyed". The principle of conservation of mass has been discovered first by the Russian scientist Mikhail Lomonosov and then Antoine Lavoisier. The mathematical representation of conservation of mass in case of fluid mechanics (Eulerian frame of reference)

\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho U) = 0
\]

2. Conservation of momentum. According to Newton's second law of mechanics, rate of change of momentum of an infinitesimal volume of fluid should equal the net forces acting on it. This simply implies that
29. The inertia forces (acceleration) should be equal in magnitude and in opposite direction of surface forces (pressure and shear) and volume or body forces (gravitational or electromagnetic).

\[ \rho U_i \frac{\partial U_i}{\partial t} + \nabla \cdot (\rho U U_i) = \rho \nabla \cdot \tau_{ij} + \rho \mathbf{e} \cdot \nabla \mathbf{e} + \rho f_i \]

3. Conservation of energy. Similar to conservation of mass, "Energy can neither be created nor destroyed; rather, it transforms from one form to another." Energy equation is direct implementation of first law of thermodynamics where the net change of energy of fluid is the difference between the gained heat and work done by its surfaces.

\[ \Phi_2 - \Phi_3 = \int \mathbf{e} \cdot \mathbf{n} \, ds + \int \frac{\partial}{\partial t} \left( \rho \mathbf{C} \right) \, ds \]

The presented Navier Stokes equations are enough to describe flow motion. However, flow may suffer chaotic behavior. This chaotic motion is called "Turbulence". Navier Stokes equations are highly nonlinear and at specific flow conditions, any small disturbance grows up tremendously (instability). In turbulent motion, a wide spectrum of flow scales exist that is why resolving all of scales of flow will be expensive computationally (using direct numerical simulation DNS).
is why it is suitable for commercial applications to model the turbulent flow in order to figure out the mean flow field parameters. Various turbulent models exist and they differ in complexity (required computational because different number of equations). The cheapest turbulent model is mixing length model (zero equations) and the most expensive is large eddy simulation, which resolves high energy eddies and models small ones. A suitable turbulent model for commercial usage is two equations model such as $\kappa$-$\epsilon$ or $\kappa$-$\omega$.

3.1.2 Turbulence Modeling

We can imagine the turbulent flow as a combination of eddies having different sizes in the flow domain. Turbulence occurs because of the instability in the flow motion. Under certain flow conditions, Navier Stokes equations become sensitive to the disturbance in the boundary conditions. It results in an amplification of the magnitude of the disturbance and chaos.

Kolmogrov performed a dimensional analysis for the turbulent flow. His main assumption is that the large eddies contain a large portion of turbulent kinetic energy and they lose it by breaking into smaller ones. Turbulent flows exhibit different length, velocity and time scales of eddies (turbulent flow exhibits highly 3D rotations) that break down transferring their energies to smaller eddies.

Any flow field property is decomposed into ensemble average and fluctuating component.

$$\phi = \phi' + \phi''$$  \hspace{1cm} (3.5)

Where $\phi$ can be velocity or pressure.
The Reynolds Averaged Navier Stokes (RANS) equations are:

\[ \bar{D}_t \bar{U}_j = \nabla^2 \bar{U}_j - \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_i} - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_j} \]

In addition, the first term can be obtained from Reynolds transport theorem:

\[ \bar{D}_t \bar{U}_j = \frac{\partial \bar{U}_j}{\partial t} + \bar{U}_i \frac{\partial \bar{U}_j}{\partial x_i} \]

The previous system of equations contains four equations; however, the number of unknowns is greater. This issue is called the closure problem. Closure problem is the need of further equations in order to be able to solve the RANS. Different models have been employed in order to model the Reynolds stresses. These models vary in the complexity and the number of equations used to capture the physics of the turbulence. The following section represents the k-\(\omega\) SST model and its equations since it is the used model in this thesis. The turbulence kinetic energy (\(k\)) and the eddy frequency (\(\omega\)) are represented through similar transport equations.
Where the model constants are $\beta^*$, $\sigma^\prime$, $\sigma^\prime\prime$, $\tau^\prime$, $\phi_1$, $\beta_1$.

Table 3.1: $k$-ω model constants

The Shear Stress Transport (SST) model is just clipping the turbulent viscosity in the turbulent sublayer through the following set of equations:

$$\min \Omega_{t,akF} \frac{\mu}{\rho} \frac{\omega}{\Omega}$$

(3.8)

$$\left( 2 \tanh F \arg \right)$$

(3.9)

$$\left( 2 \arg \max \left( \frac{\mu}{\rho}, \frac{\omega}{\Omega} \right) \right)$$

(3.10)

Vorticity magnitude

(3.11)

Boundary Conditions

In any of numerical techniques, Boundary conditions play essential role in the solution accuracy, convergence…etc. In order to have a solution that is more accurate without increasing complexity greatly, realistic boundary condition has been used. The boundary condition applied at the inlet is derived from PC-MRI using MatLab and FORTRAN codes developed by Dr. Ryo Torii [3], which compute the velocity magnitude at the inlet through specific times of cardiac cycles at some points on it. Linear interpolation has been adopted to compute the velocity at any location at the inlet at any different time. Moreover, Periodicity boundary condition has been assumed.
At the outlets of aorta, outflow boundary condition has been used that divide flow field according to certain ratios between the outlets and compute the differential pressure with respect to reference location (Outlet of descending aorta has been used as reference). The disadvantage of this assumption is that it does not take into account the compliance of aorta or time delay between blood pulse at the inlet or outlet (This delay is because of Coarctation). An extension of 5 diameters has been added to each outlet to minimize the error of the boundary condition location because vortices exist and flow is not fully developed yet so it should be trapped away. The outflow ratios have been computed by measuring mean flow at descending aorta and dividing the difference.

Table 3.2 and figure 3.1 represents the applied boundary conditions for this problem.
3.3 - Discretization and Numerical Schemes

ANSYS-CFX was used in order to model this problem. The spatial discretization scheme is high resolution. High-resolution scheme is an automatic blended scheme (between first and second order upwind). CFX tries to maximize the order of the accuracy at each time step. On the other hand, the time is discretized using second order backward scheme, which is an implicit scheme.

Velocity map at the inlet ascending descending QQ - 

Q descending and zero relative pressure
with second order accuracy. The convergence criterion is set $1 \times 10^{-5}$ for the root mean square (RMS) of the residuals. In addition, the imbalance in mass and momentum equations has been checked and found to be less than 1%.

3.4 Important parameters to quantify flow

There are a wide range of parameters that can be used in order to quantify the pulsatile flows in bends. The time-averaged wall shear stress (TAWSS), oscillatory shear index (OSI) and pressure difference have a very close understanding for clinical applications. For example, OSI affects the functionality of the endothelial cells at the wall of the aorta. Some other parameters are well understood from an engineering point of view and their impact to the human health are not established yet. The following equations report the parameters that may be used to quantify the hemodynamics.

1. Time Averaged Wall Shear Stress (TAWSS).

$$TAWSS = \frac{1}{T} \int_{0}^{T} \int_{x}^{x+1} \int_{y}^{y+1} \int_{z}^{z+1} \tau(x, y, z, t) \, dx \, dy \, dz \, dt$$

$T$ is period of cardiac cycle and $\tau(x, y, z, t)$ is instantaneous vector of wall shear stress. TAWSS represents the cardiac average of the stress at each point on the wall of the aorta.

2. Oscillatory Shear Index (OSI).

$$OSI = \frac{1}{T} \int_{0}^{T} \int_{x}^{x+1} \int_{y}^{y+1} \int_{z}^{z+1} \left( \frac{\tau(x, y, z, t)}{\tau_{max}} \right)^2 \, dx \, dy \, dz \, dt$$

OSI is an important parameter for clinical usage. It is a measure of how much wall shear stress changes its direction. It has a close connection to the functionality of endothelial cells.
3. Total Pressure

\[ \rho \left( \bar{P} + \frac{1}{2} \bar{U}^2 \right) \]

4. Kinetic Energy

\[ \rho \bar{U}^2 \]

5. Turbulent Kinetic Energy

\[ \rho \bar{U}'^2 \]

6. Turbulence Intensity

\[ \frac{\rho \bar{U}'}{\bar{U} \text{ ref}} \]

7. Strouhal Number

\[ \frac{c}{\bar{U} \text{ fl} \text{ ref}} \]

Strouhal number is an indication of the tendency of flow field to be unstable (turbulent). It is the ratio between the frequencies of the cardiac cycle and vortex shedding at specific plane inside the aorta.
Womersley Number

\[ f = \frac{\alpha v}{2} \]

Womersley number is an important parameter to judge the flow field with Reynolds number also. It represents the unsteady boundary layer thickness to the steady state boundary layer thickness. As it goes larger, the blood flow goes more stable.

Reynolds Number

\[ \text{Re} = \frac{vD}{\nu} \]

Re is the ratio between inertia forces and viscous forces.

Dean Number

\[ \text{De} = \frac{\sqrt{R \cdot \text{Re}}}{2} \]

Where \( R \) is radius of curvature of the artery. De is widely used to describe flows in bends. It represents the ratio of the square root of centripetal times inertia forces to the viscous forces. Dean number controls the behavior of the vortex at the exit of the bend.

3.5 - Grid Independence Study

Grid was obtained using ICEM CFD 15 into hexahedral bricks as shown in Figure 3. Hexahedral mesh is more preferable because it is uniform while tetrahedral causes more numerical diffusion. Moreover, for solving the same geometry we need much more tetrahedral elements than hexahedral one for the same problem with same dimensions. We discretize the domain into finite number of bricks and all of spatial derivatives such as gradient or divergence are now function of...
the grid points. As a result, a discretization error is introduced because the flow field are continuous not discrete as the solution domain.

Figure 3. Hexahedral Mesh of Aorta

The more elements we mesh, the finer resolution of the simulation. It is important to have sufficient number of elements that is capable of capturing the pattern of flow and the detailed of flow field that we are interested in. On the other hand, increasing number of elements will require a tremendous increase in the computational power. Therefore, one thing to choose the suitable grid is to run the simulation on several grids (different sizes) and compare them, which is known as grid independence study. Grid independence study was performed to make sure the global flow pattern does not change with grid size. The different size of mesh elements are 2, 4, 8, and 12 million hexa elements. The boundary layer was created using O-grid block to generate from 13 to 17 node near the wall that grows exponentially. The first wall distance was 0.01 mm and the $y+$ less than 1.3 (it should be less than 2 according to solver manual). Then, comparing the magnitude and location of maximum wall shear stress which occurs near peak systole and the maximum velocity in the shown plane through several times of the cardiac cycle. The different mesh sizes are shown in Figure 4.
The geometry of the aorta reflects various aspects of fluid mechanics besides its pulsatile nature since there might be separation bubble just at the beginning of the descending aorta due to curvature, vorticity and swirling, and the Coarctation section, which causes rapid accelerating turbulent jet in its diverging part (unstable jet). Because of all of these involved challenging physical phenomena, another plane of comparison is needed through the descending aorta. Two planes of comparison have been studied (before, and after the Coarctation) as shown in Figure 3. The third plane (plane C) has been excluded from the grid sensitivity analysis because the flow fields were stable compared to the first two planes. In addition, wall shear stress on the wall of the aorta has been analyzed to make sure it does not vary with grid size.
Figures 3.6-3.7 show the maximum velocity in each plane at different times of the cardiac cycles for the different grid sizes.
Figure 3.7 Maximum velocity at plane B for different grid sizes vs. time.

The relative difference because of grid refinement is defined to be

\[ \left| \frac{v_{\text{fine}} - v_{\text{coarse}}}{v_{\text{fine}}} \right| \times 100\% \]

where \( v \) is velocity or wall shear stress.

At the peak systole and early deceleration, velocity fields match each other with a very high precision. The maximum relative difference in the maximum velocity through plane A and B is less than 2%. On the other hand, when the velocity drops (diastole phase) the relative difference increases. It is around 5% for the last fine grids (8 and 12 M) but it reaches 17% between the coarse grids.

In addition, in peak systole, the maximum velocity is around 61 cm/sec and it drops into 9 cm/sec for the diastole. It results in that velocity scales during diastole are much smaller compared to systole (almost 0.15 the velocity at systole). Figures (3.8-3.12) represent how the maximum velocity at plane A changes with grid size at different times of the cardiac cycle.
Figure 3.8 Maximum velocity at Plane A vs. Grid size at peak systole, t=0.1 sec

Figure 3.9 Maximum velocity at plane A vs. Grid size per million, t=0.14 sec

Figure 3.10 Maximum velocity at plane A vs. Grid size per million, t=0.21 sec

Figure 3.11 Maximum velocity at plane A vs. Grid size per million, t=0.28 sec

Figure 3.12 Maximum velocity at plane A vs. Grid size per million, t=0.35 sec
Figures (3.13-3.18) shows velocity contours at different slices through different times of the cardiac cycle. In order to do verification and validation (V&V) the maximum velocity is not sufficient since in order to make sure that the mathematical model is solved correctly we have to make sure that the velocity distribution is also similar as well. Since the blood flow has pulsatile nature, various length, time, and velocity scales exist through the cycle. The following figures are taken through two planes in descending aorta in peak systole (maximum flow rate), mid-deceleration, and late diastole (aortic valve almost closed and velocity is too small). Plane A
Figure 3.14 Velocity contours at plane A, $t=0.14$ sec

Figure 3.15 Velocity contours at plane A, $t=0.21$ sec
Figure 3.16 Velocity contours at plane B, t=0.1 sec

Figure 3.17 Velocity contours at plane B, t=0.14 sec
Another important variable we need to make sure of grid independence is enough to well resolve it is wall shear stress. The variation of maximum wall shear stress on the wall of aorta because of refining grid is shown in Figure 3.19. Figure 3.19 maximum value of wall shear stress (WSS) on the wall of aorta at peak systole for different grid sizes.
Then, the location of maximum wall shear stress was investigated to make sure that it does not change which was found to be near the junction in very concentrated spot not distributed over area. The location of the nearest node that suffering maximum wall shear stress was almost the same as shown in Figure 3.

Table 3. Location of maximum wall shear stress for different grid sizes

Figure 3.21 shows the grid convergence of area averaged wall shear stress. The relative difference between the lowest and highest value is less than 1%. The contours of wall shear stress at peak systole shows that wall of aorta retained the same distribution of wall shear stress however the maximum value is almost affecting a spot or a point more than an area of the surface as shown in Figure 3.20.
Figure 3.21 Area averaged wall shear stress vs. grid size at peak systole, t=0.1 sec

Figure 3.22 Wall shear stress contours at peak systole, t=0.1 sec

The following tables summarize the results of grid independence study for the maximum velocity in the studied planes and maximum wall shear stress.
<table>
<thead>
<tr>
<th>Time</th>
<th>Plane A in Descending Aorta</th>
<th>Plane B in Descending Aorta</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Coarse(2M)</td>
<td>Medium(4M)</td>
</tr>
<tr>
<td></td>
<td>Fine(8M)</td>
<td>Finest (12M)</td>
</tr>
<tr>
<td>Difference</td>
<td>% (coarse - med)</td>
<td>% (med - Fine)</td>
</tr>
<tr>
<td>Difference</td>
<td>% (fine - finest)</td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>72.68</td>
<td>73.36</td>
</tr>
<tr>
<td></td>
<td>73.95</td>
<td>74.07</td>
</tr>
<tr>
<td>0.93</td>
<td>0.79</td>
<td>0.16</td>
</tr>
<tr>
<td>0.14</td>
<td>73.81</td>
<td>75.01</td>
</tr>
<tr>
<td></td>
<td>75.12</td>
<td>74.92</td>
</tr>
<tr>
<td>1.60</td>
<td>0.14</td>
<td>0.26</td>
</tr>
<tr>
<td>2.20</td>
<td>4.55</td>
<td>0.48</td>
</tr>
<tr>
<td>2.97</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Table 3.4</td>
<td>Maximum velocity at plane A at different times of the cardiac cycle for different grid sizes</td>
<td>Maximum velocity at plane B at different times of the cardiac cycle for different grid sizes</td>
</tr>
</tbody>
</table>
Table 3.6 Maximum wall shear stress at peak systole for different grid sizes

<table>
<thead>
<tr>
<th>Grid Size in M</th>
<th>WSS (time=0.1)</th>
<th>Relative Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>78.1376</td>
<td>4</td>
</tr>
<tr>
<td>8</td>
<td>93.743</td>
<td>5.64</td>
</tr>
<tr>
<td>12</td>
<td>97.4989</td>
<td>3.85</td>
</tr>
</tbody>
</table>

Table 3.7 Time steps for time sensitivity analysis in msec

<table>
<thead>
<tr>
<th>Large time step</th>
<th>Medium time step</th>
<th>Small time step</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 m sec</td>
<td>1 m sec</td>
<td>0.5 m sec</td>
</tr>
</tbody>
</table>

Time Sensitivity Analysis

Since the Navier Stokes equations are discretized not only in the space but in time as well because of the unsteady nature of blood flow through the aorta we have to make sure that the time step is small enough to well resolve the unsteady behavior of the flow correctly. Similarly, time sensitivity analysis was done by using twice and half the time step and comparing velocity and wall shear stress and velocity. The chosen criteria were the maximum value of wall shear stress at peak systole and maximum velocity at plane A. The following tables report the values of maximum wall shear stress at peak systole and maximum value of velocity across planes A and B at different times of the cardiac cycles. These results are plotted in Figure 3.2.
<table>
<thead>
<tr>
<th>Time Step</th>
<th>Max. Instantaneous WSS [Pa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Large</td>
<td>93.17</td>
</tr>
<tr>
<td>Medium</td>
<td>93.74</td>
</tr>
<tr>
<td>Small</td>
<td>92.87</td>
</tr>
</tbody>
</table>

Table 3.8

Max. Wall shear stress at peak systole for different time step sizes

<table>
<thead>
<tr>
<th>Time Step</th>
<th>Error Large-Medium [Pa]</th>
<th>Error Medium-Small [Pa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Large</td>
<td>0.10</td>
<td>0.18</td>
</tr>
<tr>
<td>Medium</td>
<td>0.14</td>
<td>0.21</td>
</tr>
<tr>
<td>Small</td>
<td>0.21</td>
<td>0.28</td>
</tr>
</tbody>
</table>

Table 3.9

Max. Velocity at plane A for different time step sizes at different times of the cardiac cycle

Figure 3.23

Max. Wall shear stress vs. time
In order to validate the results of the numerical simulations, comparisons with PC-MRI were held. We have the data at the descending aorta only for one case. The maximum normal velocity across that plane is compared and found that it differs by 10% at peak systole. The following figure 3.24 shows the location of the plane used for validation and contours of normal velocity across the plane of validation.

Figure 3.24 Validation of the normal velocity obtained by PC-MRI (left) and CFD (right).


4. Results and Discussion.

4.1 Introduction.

This section discusses and shows the results of numerical simulations of both pre-operative and post-operative cases through different scales of analysis starting by qualitative analysis, which depends on the big picture noticing similarities and differences between the simulation and reported normal healthy people and then going deeper quantifying important numbers that can correlate the results of CFD to practical uses. Finally, a study of the sensitivity to the complexity of modeling on the results has been performed.

The five patients have significantly different geometries and other different medical problems. The five cases are labeled as following: The first patient is MAT, the second patient is OA, the third patient is OMM, the fourth patient is OMW and the fifth patient is YAB. The first case (MAT) exhibits a narrow area just after the inlet of the aorta. Moreover, this case did not suffer CoA only but also the pulmonary and aorta artery were exchanged. The third case (OMM) represents a large angulation of the outer surface of the aorta. The fourth case (OMW) shows a dilation after the surgery in the area of treatment. The fifth case (YAB) doesn't only suffer CoA but a bicuspid aortic valve (BAV) as well which has a significant effect on the hemodynamics.

4.2 Flow pattern in healthy aorta.

In healthy or normal aortas, Kilner described flow pattern as follows:

1. In acceleration phase well-structured flow attached to the direction of vessel with max. velocity near to the inner wall of ascending aorta.

2. In deceleration phase vortices and helical structures are developed. The helical motion is right handed in the arch and left handed helical motion through distal aorta.

3. In late diastole: laminar vortices with small velocities.
The first investigation is based on the qualitative analysis, which can describe the evolution of hemodynamics across aorta and the similarities between preoperative as a group and postoperative as another group and the differences between them. Qualitative analysis is done by showing important contours of parameters of interest; velocity (streamlines and velocity vectors), pressure difference, structure of vortices, and time averaged wall shear stress (TAWSS) in order to distinguish the flow pattern in preoperative and postoperative.

1. Streamlines/velocity vectors. In order to visualize flow formation “Velocity Profile”, flow pattern, areas of separation and back flow.

2. Areas suffering high rotations. To visualize vortices and their types in aorta because certain flow motions exist because of Coarctation. There are different types of vortex regions such as vortex rings, horseshoe, vortex tube, and span wise vortex regions.

3. General analysis of TAWSS. TAWSS is an important biomarker and indication to compare between different patients and normal ones. The rupture of aorta occurs mainly because of shear stress however, its time averaged magnitude is very low compared with pressure values.

4. Pressure difference. The recurrence of CoA usually happens when the pressure drop exceeds 20 mmHg. This procedure will be applied at accelerating and decelerating phases.
Figure (4.1) shows the distribution of time averaged wall shear stress on the wall of aorta. The pre-operative cases are shown on the first row. For healthy aorta, TAWSS is in order of 1 pascal. Both pre-operative and post-operative suffer high wall shear stress at the branching points because of the high strain rate to divide flow between branches. In addition, both pre-operative and post-operative showed sensitivity to the inlet boundary conditions and the geometry of the arch. For example, case C exhibited a high-speed jet hits the wall of the ascending aorta which resulted at a very high TAWSS. For pre-operative simulations, concentrated higher wall shear stress is around the area of Coarctation itself. Only one case has almost zero wall shear stress because the flow rate was very small (almost stagnant). For post-operative, wall shear stress is obtained in range of 1.5 pascal except in one case that suffered very large rotational motion resulted in very high stress larger than 5 Pascal. This is also due to the inlet boundary condition where there is malfunction at the aortic valve making such skew velocity profile towards the wall of aorta.
Figure 4.1 TAWSS for both of pre-operative (top) and post-operative (bottom).

1. Concentrated TAWSS due to narrowed areas,
2. Impingement,
3. High TAWSS on the whole wall.

Figure 4.2 shows the streamlines at peak systole. Pre-operative, the main difference lies in the formation of the jet that hits the wall of the aorta. Also, backflow after area of Coarctation and reattachment later. The abrupt narrowing of the area in the aorta results in increasing the velocity magnitude and when the area is large again vortices, backflow, and instability occurs. For post-operative the first case has highly disturbed flow because of pre-ductal Coarctation. They also showed well-structured attached flow to the direction of the vessel through the arch and descending aorta. The inlet velocity at the third case hits the outer wall of the arch, which caused the high shear stress because of the angle between the peak velocity magnitude and the centerline of the aorta.

The last case has very high velocity (150 cm/sec) beside the start of development of helical motion. In general, separation bubble exists also at the beginning of the descending aorta (end of the arch).
Figure 4.2 Streamlines colored by velocity magnitude at peak-systole for both pre-operative (top) and post-operative (bottom).

1. Jet formation
2. Impingement

Figure (4.3) shows the streamlines in mid-systole, both pre and post-operative cases showed highly disturbed flow influenced by either geometry or inlet velocity profile. For pre-operative the jet formation because of the narrowing in geometry still exists beside backflow at the area of Coarctation followed by destruction in flow shape. Only first case is different because of different geometry caused the flow to be in the direction of the vessel again. For post-operative, the first case had a pre-ductal Coarctation caused disturbed flow conditions at the inlet resulted in chaotic motion. The second treated case did not show helical motion. On the other hand, the third arch still suffers because of the hit of high jet of inlet at the wall of ascending aorta while flow profile in descending aorta is better. The flow profile in fourth case tried to develop helical motion however some disturbance still exists because of the difference of area in distal aorta but flow profile after short distance is attached to the vessel direction again. The last case has very high velocity (around 100 cm/sec).
Figure 4.3 Streamlines colored by velocity magnitude at mid-systole for pre-operative (top) and post-operative (bottom).

Figure (4.4) shows the vortex core regions according to lambda2 criterion at level of 0.01 colored by the percentage of turbulence intensity. Lambda2 is a method used to detect coherent structures and continuous vortices. Each point lies in the vortex core if its lambda2 is negative. Lambda2 is the second eigenvalue of the following tensor (H):

\[
\begin{align*}
J &= \nabla \bar{U} \\
S &= \frac{1}{2}(J + J^T) \\
\Omega &= \frac{1}{2}(J - J^T) \\
H &= S^2 + \Omega^2
\end{align*}
\]
For preoperative cases, they exhibited vortex rings at the entrance (valve level) and after Coarctation as well. Vortex rings occur usually because of change of area. The fourth case presented vortex tube from ascending till descending of aorta which represents the vortex structures through bulk flow. For the postoperative cases, the first case presented also vortex ring at the preductal Coarctation, the third case showed horsehoe vortex core region because of when the jet hits the wall it reflects away, and the fifth case showed vortex tube. All of the cases exhibited span wise vortex regions near the wall and less stream wise.

Figure 4. Vortex core regions at peak-systole obtained by lambda2 colored by turbulence intensity percentage for preoperative (top) and postoperative (bottom).
regions. Turbulent intensity is high in the first post-operative arch, third one pre and post-operative as well through ascending aorta.

Figure 4.5 Vortex core regions at mid-late systole colored by turbulence intensity percentage for pre-operative (top) and post-operative (bottom)
Figures (4.6) and (4.7) show the pressure at peak systole and mid late systole both pre and post operative presented pressure difference no more than 10 mmHg that guarantees no recurrence of Coarctation to occur.

Figure 4.6 Relative pressure to the outlet of descending aorta on the wall at peak systole for preoperative (top) and postoperative (bottom)
Figure 4. Relative pressure to the outlet of descending aorta on the wall at mid-systole for pre-operative (top) and post-operative (bottom)
4.4 Quantitative Analysis

The second step will be to perform numerical assessments of important parameters to quantify flow dynamics. This is done by plotting kinetic energy across centerline, Strouhal number, amount of backflow of total flow rate and local indices of TAWSS. It should be noticed that some engineering parameters: turbulent kinetic energy (TKE), Womersley number and Strouhal number, used in the provided analysis are under research in order to establish their clinical relevance.

a. Analyzing global indices of hemodynamics such as maximum velocity at peak systole and time averaged wall shear stress TAWSS. Table (4.1) reports the maximum TAWSS acting on the wall of aorta, area averaged TAWSS and how percentage of the area of aorta is under different levels of stresses. Three levels have been chosen: above 5 pascal, between 1 and 5 pascal, and less than 1 pascal. In addition, the maximum velocity in the arch across the cardiac cycle is reported as well. The no-slip condition at the walls is the reason for the wall shear stress exerted by a fluid. Wall shear stress is proportional to the velocity gradient at the wall and the viscosity of the fluid as well. Velocity gradient is affected largely by the shape or the geometry such as bends will produce separation, the vortices due to secondary flow, area narrowing, or irregularities of the wall. In addition, increasing flow rate results in an increase in wall shear stress. That's why wall shear stress is an important parameter that relates geometry and flow rate together beside its impact on the mechanics of the wall since rupture may occur in case of excessive shear stresses.

The first case presents an increase of the maximum velocity in the whole aorta by factor of 3.69 after treatment with respect to preoperative (133 cm/sec in post-op and 36 cm/sec in pre-op) and with factor of 5.45 for max. Flow rate ratio (from 11 ml/sec in pre-operative to 66 ml/sec in post-op)
operative). Both maximum TAWSS and area averaged TAWSS show a significant increase from 3.9 pascal to 20.9 pascal and from 0.17 pascal to 1.24 pascal by factors of 5.3 and 7.3. In case of pre-operative, 99.5% of the area suffered TAWSS less than 1 pascal and 0.5% of the area was exposed to TAWSS between 1 pascal and 5 pascal. After the surgery, 60.5% of the wall remained under TAWSS less than 1 pascal, 36.5% between 1 pascal and 5 pascal, and 3% of the area suffers more than 5 pascal. The reason for the jump in max. TAWSS is a very large flow rate and velocity pass through a narrow area after the inlet directly.

The second case shows different behavior by a decrease in the maximum velocity through the whole aorta as it was 98.5 cm/sec in pre-operative and became 70 cm/sec after treatment, which means a decrease in maximum velocity by factor of 1.4 however the flow rate increased by factor of 2.2 (from 25 ml/sec in pre-operative to 55 ml/sec in post-operative). The max. TAWSS shows a decrease from 16.7 pascal to 9.9 pascal. On the other hand, area averaged TAWSS increased from 0.62 pascal to 0.73 pascal however; both of values are low with respect to other cases either pre-operative or post-operative. The distribution of TAWSS on the wall of aorta does not vary between the two cases significantly as the area exposed to TAWSS less than 1 pascal represents 85.7% in pre-operative and 80.6% after surgery. The percentage of the area exposed to TAWSS between 1 pascal and 5 pascal is 13.42% in pre-operative and 19.15% after surgery. Both simulations show a very small amount of the area of the arch is under TAWSS larger than 5 pascal as it is 0.85% in pre-operative and 0.25% after surgery. The decrease in TAWSS is explained by removing the effect of the jet (Coarctation) since the highest value in pre-operative was due to the narrow area in descending aorta so the maximum velocity is less and the area is larger in post-operative.
In the third case, both maximum velocity and max. Flow rate are larger in post-operative compared with pre-operative. For maximum velocity, it is 165 cm/sec in case of pre-operative and 192 cm/sec after treatment while the volumetric flow rate shows an increase from 60 ml/sec in pre-operative to 100 ml/sec in post-operative. The max. TAWSS presents slight increase from 16.1 pascal to 18.8 pascal after surgery however, the area averaged TAWSS shows a decrease from 1.61 pascal to 1.56 pascal. The distribution of TAWSS on the wall of aorta shows that the area exposed to TAWSS less than 1 pascal is 44.8% in pre-operative and 55% after treatment but the area exposed to TAWSS between 1 pascal and 5 pascal shows a decrease from 51.5% in pre-operative to 38.9% in post-operative. The percentage of area that suffer TAWSS larger than 5 pascal shows an increase from 3.6% to 6%. The reason behind this increase is the increase of the velocity jet hitting the wall, which is causing the significant amount of high TAWSS in this case.

The fourth case does not show an increase in maximum velocity as it remained 133 cm/sec pre and post the operation but the max. Flow rate shows an increase from 44 ml/sec to 87 ml/sec. The max. TAWSS is 24.7 pascal in pre-operative and 33.2 pascal after treatment showing an increase however, no significant change in the area averaged TAWSS since it is 1.78 pascal in pre-operative and 1.73 in post-operative. The TAWSS distribution has an increase in the area subjected to TAWSS less than 1 pascal to be 38.5% in post-operative instead 28.47% in pre-operative, decrease in the percentage of area subjected to TAWSS between 1 pascal and 5 pascal to be 58.27% in post-operative instead 69.7% in pre-operative, and an increase in the percentage of the area subjected to TAWSS more than 5 pascal to be 3.2% in post-operative than 1.8% in pre-operative. The area subjected to TAWSS increased because of removing the narrowing in downstream however, in same time the area subjected to high TAWSS larger than 5 pascal because of the effect of the jet hitting the wall of ascending aorta as in third case.
The fifth case shows the most varied result among the results concerning TAWSS distribution. First, the maximum velocity is 161 cm/sec in post-operative larger than in pre-operative (118 cm/sec). In addition, volume tric flow rate shows an increase to be 82 ml/sec in post-operative than 35 ml/sec in pre-operative. Both pre-operative and post-operative have near max. TAWSS values 21 pascal and 26 pascal in turn. The area averaged TAWSS in post-operative is 3.7 pascal larger than in pre-operative (1.7 pascal). The distribution of TAWSS on the wall of aorta shows great significant difference between the two cases. The percentage of the area under TAWSS less than 1 pascal in pre-operative is 40% and 17% in case of post-operative, the percentage of area under TAWSS between 1 pascal and 5 pascal in pre-operative is 55% and 53% for post-operative, and concerning the percentage of area subjected to excessive TAWSS larger than 5 pascal, it is 4.5% in pre-operative and 26.5% in post-operative. The explanation to this jump is the effect of the inlet boundary condition as shown in the following figure (4.8), the maximum velocity is so near to the wall resulting in a very high velocity gradient and very small boundary layer thickness. In addition, this resulted in very aggressive helical motion downstream and very large shear strain rate.

Figure 4.8 the inlet velocity profile in both CFD and PC-MRI.
The following figure (4.9) visualizes the previous table (4.1) by showing the percentage of the area subjected to certain amount of TAWSS or less. For preoperative cases, it can be judged that the aorta is exposed to almost same amount of TAWSS except some certain spots. After surgery, the load or stress is distributed wall not concentrated on specific spots. Also, it can be noticed the shift in the distribution of TAWSS for the fifth case which suffered excessive stresses i.e., a very large portion of the area is exposed to high stress (line is shifted to right). The second figure (4.10) shows that the absolute amount of area exposed to specific value of WSS increased after surgery. In other words, the shear force on the wall of aorta after surgery has increased.
Figure 4.9 the cumulative distribution of percentage of area vs. TAWSS for pre-operative (left) and post-operative (right).

Figure 4.10 the cumulative distribution of area in mm$^2$ vs. TAWSS in pascal for pre-operative (left) and post-operative (right).
Table (4.2) reports the area of the inlet and Womersley number. Both areas have increased after surgery. The increase of inlet area will result in an increase in the mass flow rate and Reynolds number as well. Womersley number is a measure of the transient forces to viscous forces. It increases proportionally with the diameter or the square root of frequency of cardiac pulse. The lower Womersley number, the more steady flow exists and a parabolic shape velocity profile exists. When the Womersley number is high, it means high pulsatility or frequency with almost flat velocity profile shape.

<table>
<thead>
<tr>
<th>Case</th>
<th>Pre-Operative</th>
<th>Post-Operative</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAT</td>
<td>99.84</td>
<td>250.33</td>
</tr>
<tr>
<td>OA</td>
<td>58.9</td>
<td>222.8</td>
</tr>
<tr>
<td>OMM</td>
<td>207.14</td>
<td>229.8</td>
</tr>
<tr>
<td>OMW</td>
<td>107.13</td>
<td>164.66</td>
</tr>
<tr>
<td>YAB</td>
<td>111.4</td>
<td>133.2</td>
</tr>
</tbody>
</table>

Table 4.2: Area of the aortic inlet and Womersley number
Figure 4.11 Womersley number for the different cases

Figures (4.12) shows the Reynolds number at the inlet of aorta. It increased in all cases for post-operative compared with before the surgery. This increase is due to an increase in the area of the inlet (diameter) and the increase of the mass flow rate (mean velocity) that enters aorta. It means that we have more energy or momentum in the blood flow (more efficient pump).
Figure 4.12 Reynolds number for the different cases: (a) preoperative, and (b) postoperative.

Quantification of Improvement by comparing amount of backflow, WSS and TKE. The following charts in figure (4.13) represent specific turbulent kinetic energy plotted in a log scale across the cardiac cycle. All of the postoperative cases have higher amount of turbulence than preoperatives. The tremendous increase in the flow rate (higher Reynolds number) without any change in the regions of ascending aorta having very disturbed flow pattern resulted in increasing the losses in terms of specific turbulence kinetic energy.

$$\text{STKE} = \rho V^2$$
Figure 4.13 Specific turbulent kinetic energy: (a) MAT, (b) OA, (c) OMM, (d) OMW, and (e) YAB

The following figure (4.14) shows the distribution of the wall shear stress and the amount of blood flow in the direction of the vessel. By obtaining the centerline of the aorta, several cross-sections normal to it have been taken. The wall shear stress at the peak systole has been averaged on the
The amount of velocity is then resolved into two components: normal to the cross-section and in plane. The amount of velocity normal to the cross-section means that blood flow is attached to the direction of the aorta and a small portion of the energy is wasted in vortices. The sections that are suffering very disturbed flow nature show a drop in the amount of normal velocity reaching a value around 40% of the area-averaged velocity across the cross-section. At these areas of rotations, the maximum amount of wall shear stress occurs due to the high shear strain. After the surgery, there is an improvement in the flow pattern in the descending aorta even though the disturbance of blood flow still exists in the upper stream (ascending aorta).
Figure 4.14 Length averaged wall shear stress (WSS) and velocity alignment (α) across the normalized distance of the centerline of the aorta: (a) MAT, (b) OA, (c) OMM, (d) OMW, and (e) YAB.
Strouhal number is a non-dimensional parameter indicating the possibility that instability may occur in the flow. It represents the ratio of time scale (or frequencies) at some location in the aorta and the global time scale of the problem. The cardiac time is used as reference time. Strouhal number was calculated at plane in descending aorta in the same level of the inlet. Figure (4.15) shows the location used to calculate Strouhal number. Table (4.3) and Figure (4.16) reports the values of Strouhal number. All pre-op simulations exhibit higher Strouhal number than after surgery except for the fourth case (OMW). The flow tends to be laminar and steady when Strouhal number is low. Strouhal number is a measure of the frequency of the vortices.

<table>
<thead>
<tr>
<th>Case</th>
<th>Pre-Op</th>
<th>Post-Op</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAT</td>
<td>0.126</td>
<td>0.0382</td>
</tr>
<tr>
<td>OA</td>
<td>0.1226</td>
<td>0.069</td>
</tr>
<tr>
<td>OMM</td>
<td>0.0567</td>
<td>0.0361</td>
</tr>
<tr>
<td>OMW</td>
<td>0.0635</td>
<td>0.0858</td>
</tr>
</tbody>
</table>
In this section, both global and local parameters are studied and analyzed in order to optimize the computational cost without affecting the solution significantly. The computational cost is proportional to the physics involved in the simulation. Turbulent simulation takes more time to be resolved because of the addition of turbulence model equation (two equation in this case) beside its fine mesh requirement. Non-Newtonian viscosity model also results in a more complex simulation.
The three cases differ in the Reynolds number, cardiac frequency and in the geometry. According to figures (4.17) and (4.18), the Reynolds number is 268, 741 and 1294. The Womersley number is 7.5, 9.2 and 9.1 according to table (4.2). Finally, it can be seen there is large difference between the geometry of the cross-section between the three cases. The first two arches have almost circular cross-section however, the third one has an oval profile.

Table (4.3) reports the area averaged time averaged wall shear stress for the different simulations (laminar Newtonian, laminar non-Newtonian, turbulent Newtonian and turbulent non-Newtonian) of three patients (pre-operative). Table (4.4) presents the maximum value of the TAWSS on the whole surface of the aorta and table (4.5) reports the maximum value of the velocity magnitude in the domain (volume) of the aorta all over the cardiac cycle.

**Table 4.4 Area-averaged of the time averaged wall shear stress at different viscosity and flow regime models**

<table>
<thead>
<tr>
<th>Model Type</th>
<th>MAT</th>
<th>OAM</th>
<th>OMM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laminar Newtonian</td>
<td>2.288</td>
<td>0.662</td>
<td>1.63</td>
</tr>
<tr>
<td>Laminar Non-Newtonian</td>
<td>2.294</td>
<td>0.664</td>
<td>1.631</td>
</tr>
<tr>
<td>Turbulent Newtonian</td>
<td>1.911</td>
<td>0.623</td>
<td>1.613</td>
</tr>
<tr>
<td>Turbulent Non-Newtonian</td>
<td>1.92</td>
<td>0.625</td>
<td>1.611</td>
</tr>
</tbody>
</table>

Figure 4.17 Location of the plane and lines used in the analysis. Figure 4.18 The centerline of the aorta...
Table 4.5 Maximum time averaged wall shear stress at different viscosity and flow regime models

<table>
<thead>
<tr>
<th>Model</th>
<th>Laminar</th>
<th>Newtonian</th>
<th>Non-Newtonian</th>
<th>Turbulent</th>
<th>Newtonian</th>
<th>Non-Newtonian</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAT</td>
<td>3.896</td>
<td>3.91</td>
<td>3.924</td>
<td>3.93</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OA</td>
<td>15.65</td>
<td>15.65</td>
<td>16.68</td>
<td>16.68</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OMM</td>
<td>15.44</td>
<td>15.44</td>
<td>16.146</td>
<td>16.11</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 4.6 maximum velocity magnitude across the cardiac cycle at different viscosity and flow regime models

The previous tables (4.4, 4.5 and 4.6) did not show any significant change between the estimation of the global values of flow fields; area averaged TAWSS, maximum TAWSS or the maximum velocity. The velocity was compared at a plane downstream the area of Coarctation as shown in figure (4.18). The velocity magnitude is plotted over two perpendicular lines on the same plane as shown in figure (4.18) besides plotting it across the centerline of aorta as shown in figure (4.17). Two instances of the cardiac cycle have been chose; peak systole since the flow is its maximum velocity and maximum deceleration since there is helical motion at large velocity as well.

There is no visual difference in the velocity magnitude or the in-plane vectors at the peak systole. However, when the blood flow starts to decelerate the velocity vectors and its magnitude differ. The first case, which has almost circular cross section, low Re and low Womersley number, shows the same distribution. The second case, which has medium Re and higher Womersley number,
shows no difference in the peak systole. At the deceleration, both of laminar simulations overestimated the maximum magnitude of the velocity. On the other hand, the last case which has complex geometry, high Re and Womersley numbers shows also the same distribution in case of peak systole but major differences between the four simulations in case of deceleration. The shape of the vortices differed. The laminar model overestimated the peak velocity as well.

The following figure (4.19) shows the velocity magnitude and the inplane velocity vectors at four conditions: laminar Newtonian, laminar non-Newtonian, turbulent Newtonian and turbulent non-Newtonian at two times of the cardiac cycle: peak systole and mid deceleration.
The following figures (4.20, 4.21 and 4.22) show the velocity across two perpendicular lines on the previous plane of study and the centerline of the vessel where horizontal line is L1, vertical line is L2 and the centerline is CL. The velocity magnitude for the first case was the same for both peak systole and mid-to-late diastole for all simulations. On the other hand, the in-plane velocity magnitude differed for the second and third cases. The difference is due to the flow regime model mainly (laminar or turbulent) not the viscosity model (Newtonian or non-Newtonian). The laminar model overestimates the maximum velocity. Turbulent models are assuming a higher viscosity and a better mixing. It results in a more diffusive flow pattern. Laminar model of the flow fields assume no turbulence losses and it tries to model the turbulent eddies as laminar ones resulting in higher velocity magnitude.
Figure 4.20 Velocity magnitude at two slices of time: peak systole (left) and mid-deceleration (right) across L1 (top), L2 (middle) and CL (bottom) for the first pre-operative case (MAT).
Figure 4. 21 Velocity magnitude at two slices of time: peak systole (left) and mid-deceleration (right) across L1 (top), L2 (middle) and CL (bottom) for the second pre-operative case (OA).
Figure 4.22 Velocity magnitude at two slices of time: peak systole (left) and mid-deceleration (right) across L1 (top), L2 (middle) and CL (bottom) for the third pre-operative case (OMM).
Conclusion
Several research showed that combining both medical and engineering knowledge is able to lead to a better understanding of the diseases and improving the methods for treatment and surgeries. For example, CFD is widely used to design stents, ventricular assist devices…etc. Merging the current technologies in hospitals (imaging techniques) and numerical techniques (CFD) managed to investigate the abnormal hemodynamics that is resulting from cardiovascular diseases.

This research focuses on investigating the hemodynamics for patients with CoA (pre and post-operative). The objectives were to investigate the blood flow patterns, quantify the improvement and estimating the sensitivity of the simulations to different modeling parameters.

A real geometry of five patients were numerically studied using ANSYS CFX. The boundary conditions at the inlet were driven from PC-MRI and mapped to the numerical domain. All of the cases were modeled as turbulent using k-ω SST model because of its capabilities to capture near-wall physics. The blood was modeled to be Newtonian (constant viscosity 4 mpa.sec). A further step was to identify how the simulation results vary with respect to the model parameters. Three pre-operative patients with different Reynolds and Womersley numbers were chosen and simulated with four conditions (turbulent Newtonian, turbulent non-Newtonian, laminar Newtonian and laminar non-Newtonian). Carreau-Yasuda model was used to model the non-Newtonian viscosity of the blood.

The geometry showed a significant effect on the flow fields. The angle between the outer surface of the aorta and the velocity vector was responsible for producing an impingement, which caused a very large TAWSS affecting a large area of the ascending aorta. Moreover,
when the ascending aorta was almost vertical, large amount of blood flow with large velocity flowed towards the neck vessels.

- Numerical simulations are important to quantify the improvement and find the locations that should be examined after the CoA surgery. A simple measure of the improvement is the ratio between the amount of velocity in the direction of the vessel to the magnitude of the velocity vector. This shows how much energy is wasted in vorticity or the backflow.

- Hemodynamics in aorta is in transitional regime. In addition, it is important to consider the blood as a non-Newtonian fluid in case of low velocities. However, applying different simulations parameters showed that the turbulence effects are more important than the viscosity ones. In addition, the results obtained that the turbulence model is important to capture the physics near the wall and has a large effect on the velocity field.

Recommendations for future work

- Using the numerical techniques can be used as a decision assistant tool for physicians to simulate different virtual surgeries and select the proper one.

- Development of a reduced order model is needed to predict the increase in mass flow rate after the surgery. This can be used as a boundary condition for simulating the virtual surgery.