

São Paulo State University
School of Natural Sciences and Engineering

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**Hemodynamic changes in intracranial
aneurysms due to stent-induced vascular
remodeling**

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Hemodynamic changes in intracranial aneurysms due to stent-induced vascular remodeling

Thesis submitted to the School of Natural Sciences and Engineering of the São Paulo State University (UNESP) in partial fulfillment of the requirements for the degree of Master of Sciences in Mechanical Engineering. Field of Thermal Sciences.

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Dedicated to my parents: Milton and Solange.

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ABSTRACT

Stents were first designed to act as mechanical barriers, preventing coil herniation into the parent artery. The current generation of self-expanding intracranial stents has recently been shown to change the local vascular geometry, a phenomenon with unclear hemodynamic effects. We carried out numerical simulations to assess the role of stent-induced vascular remodeling in modifying intraaneurysmal hemodynamics. Simulations were performed using the open-source software OpenFOAM. Blood was assumed to behave as an incompressible Newtonian fluid; vessel walls were assumed to be rigid. Wall shear stress, WSS, and oscillatory shear index, OSI, were evaluated to quantify the hemodynamic changes in the aneurysm sac. Four pre- and post-stent patient-specific geometries of intracranial bifurcation aneurysm were used. In one aneurysm at the anterior communicating artery (ACoA) bifurcation, a single stent was deployed, resulting in straightening of the host vessels. After stenting, WSS and OSI increased by approximately 60% and 25%, respectively. In two aneurysms at middle cerebral artery (MCA) bifurcations, two stents in a “Y” configuration were deployed, resulting in straightening of both daughter arteries. The maximum WSS on the aneurysm surface increased by approximately 5% in one case and 22% in the other. In another aneurysm at a bifurcation of the MCA, a single stent was deployed, resulting in straightening of the host vessels. After stenting, WSS and OSI reduced by approximately 13% and 50%, respectively. The results show that hemodynamic changes do occur in intracranial bifurcation aneurysms due to stent-induced vascular remodeling. Contrary to previous suspicions, the effects of stent-induced vascular remodeling in modifying the intraaneurysmal hemodynamics are variable and not always beneficial. In conclusion, stent-assisted treatments of bifurcation aneurysm such as two-step Y-stent coiling may benefit from the novel vascular geometry by placing a single stent in an earlier step. However, a two-step procedure would not be recommended for aneurysms at the ACoA bifurcation, where straightening of the host vessels may cause an adverse hemodynamic environment and increase the risk of rupture.

Keywords: Intracranial aneurysms. Stents. Vascular remodeling. Computational fluid dynamics. Hemodynamics.

RESUMO

Originalmente, *stents* foram projetados para agir como barreiras mecânicas, impedindo a herniação de coils para a artéria-mãe. Recentemente, estudos mostraram que a atual geração de *stents* intracranianos auto-expansíveis altera a geometria local das artérias: um fenômeno com efeitos hemodinâmicos em parte incompreendidos. Nós realizamos simulações numéricas para avaliar a influência da remodelagem arterial induzida por *stent* sobre a hemodinâmica em aneurismas intracranianos. As simulações foram realizadas utilizando o *software open-source* OpenFOAM. O sangue foi modelado como fluido Newtoniano incompressível e as paredes arteriais foram consideradas rígidas. Para quantificar as alterações hemodinâmicas, avaliamos os parâmetros *wall shear stress*, WSS, e *oscillatory shear index*, OSI. Quatro geometrias reais de aneurismas intracranianos em bifurcações foram utilizadas. Em um aneurisma na bifurcação da artéria comunicante anterior (ACoA), um *stent* foi implantando, levando ao endireitamento das artérias que o receberam. Após o procedimento, os níveis de WSS e OSI aumentaram aproximadamente 60% e 25%, respectivamente. Em dois aneurismas em bifurcações da artéria cerebral média (MCA), dois *stents* foram implantados em uma configuração em “Y”, resultando em um endireitamento de ambas as artérias-filhas. O WSS máximo na superfície do aneurisma aumentou aproximadamente 5% em um dos casos e 22% no outro. Em outro aneurisma em uma bifurcação da MCA, um *stent* foi implantado, resultando no endireitamento das artérias que o receberam. Após o procedimento, valores de WSS e OSI sofreram uma redução de aproximadamente 13% e 50%, respectivamente. Os resultados mostram que alterações hemodinâmicas de fato ocorrem em aneurismas intracranianos em bifurcações devido à remodelagem arterial induzida por *stents*. Em contraste com suspeitas anteriores, os efeitos da remodelagem arterial induzida por *stents* sobre a hemodinâmica de aneurisma apresentam um comportamento variável e nem sempre benéfico. Concluímos, portanto, que a remodelagem arterial induzida por *stents* pode beneficiar tratamentos de aneurismas intracranianos, como o procedimento em dois tempos de “Y-*stent coiling*”, através do implante de um único *stent* em uma etapa prévia. No entanto, procedimentos em dois tempos não seriam recomendado para aneurismas na bifurcação da ACoA, onde o endireitamento das artérias pode causar uma resposta hemodinâmica adversa e aumentar o risco de ruptura do aneurisma.

Palavras-chave: Aneurismas intracranianos. *Stents*. Remodelagem arterial. Mecânica dos fluidos computacional. Hemodinâmica.

LIST OF FIGURES

Figure 1 – Schematic illustration of (a) bifurcation and (b) sidewall aneurysms. . .	17
Figure 2 – Inferior view of the base of the brain showing an interconnected circulatory structure composing the circle of Willis—internal carotid arteries (ICA) and their branches: middle cerebral arteries (MCA) and anterior communicating arteries (ACA); the vertebrobasilar system, composed of the vertebral arteries (VA) and the basilar artery (BA); and the anterior communicating artery (ACoA), connecting the left and right branches of the ACA.	18
Figure 3 – Schematic illustration of coiling techniques: (a) stand-alone coil embolization and (b) stent-assisted coil embolization.	19
Figure 4 – Schematic illustration of a shape-memory alloy stent subject to a bending angle θ . $\mathbf{F}_{bending}$ is a resulting counteracting force dependent on θ and $\mathbf{F}_{radial}$ is an ever-present outward-directed radial force as a result of the self-expanding design of the stent.	21
Figure 5 – Blood flow rate for the internal carotid artery (ICA) normalized with respect to the temporal mean blood flow rate.	24
Figure 6 – Mean blood flow rate through the arteries of the brain as a percentage of the total blood flow rate reaching the brain: (11.95 ± 2.05) ml/s. . .	25
Figure 7 – Volume rendering representation of a 3DRA image file. Picture taken using the visualization software ParaView.	26
Figure 8 – Volume rendering representation of a 3DRA image file. Volume of interest (VOI) enclosing the aneurysm and its surrounding vessels. Picture taken using the visualization software ParaView.	27
Figure 9 – Volume rendering representation of a 3DRA image; blue surface highlights the final aneurysm surface reconstructed using VMTK utilities. Picture taken using the visualization software ParaView.	28
Figure 10 – Reconstructed surfaces of case 11, case 16, case 17, and case E1. Red lines illustrate where stents were deployed.	29
Figure 11 – Arbitrary polygonal control volume V_C with centroid C of a 2D finite volume mesh, and its neighboring cells with centroid F_i	30
Figure 12 – Speedup, s , as a function of the number of processors, N , for the pre-stent geometry of case 11.	35

Figure 13 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case 11 at systolic peak; A and B indicate the flow impingement zone at the dome of the aneurysm and a large area of low WSS ($WSS < 1.5$ Pa), respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surface: 28 Pa and 6.3 versus 29.3 Pa and 7.2, respectively.	37
Figure 14 – Flow pattern in the (a) pre-stent and (b) post-stent geometries of case 11 at systolic peak.	38
Figure 15 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case 11; A and B indicate high OSI values coinciding with the flow impingement zone at the dome of the aneurysm and a large area of low WSS, respectively. Maximum and mean OSI on the pre- and post-stent aneurysm surfaces: 0.46 and 0.042 versus 0.41 and 0.024, respectively.	38
Figure 16 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case 16 at systolic peak; A and B indicate a low WSS region on the pre- and post-stent surfaces, respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surfaces: 47.3 Pa and 15 Pa versus 57.7 Pa and 17.1 Pa, respectively.	39
Figure 17 – Flow pattern in aneurysm case 16 at systolic peak: (a) side view of the pre-stent geometry and (b) frontal view of the post-stent geometry. Points A and B indicate a slow recirculation flow causing a low WSS region on both surfaces.	40
Figure 18 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case 16. Point A indicates elevate OSI levels coinciding with a low WSS region ($WSS < 1.5$ Pa). Maximum and mean OSI on the pre- and post-stent aneursym surfaces: 0.32 and 0.007 vs 0.40 and 0.008, respectively.	41
Figure 19 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case 17 at systolic peak; A and B indicate areas of low and high WSS on the aneurysm sac, respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surfaces: 49.4 Pa and 11.5 Pa versus 81.2 Pa and 18.5 Pa, respectively.	41
Figure 20 – Flow pattern in the (a) pre-stent and (b) post-stent geometries of case 17 at systolic peak.	42
Figure 21 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case 17. Maximum and mean OSI on the pre- and post-stent aneursym surfaces: 0.34 and 0.012 versus 0.37 and 0.015, respectively.	42

Figure 22 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case E1 at systolic peak. Point A and B indicate a region of high WSS due to flow impingement against the aneurysm neck and a region of high WSS on the aneurysm dome, respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surfaces: 77.3 Pa and 10.8 Pa versus 47.4 Pa and 9.4 Pa, respectively.	43
Figure 23 – Flow pattern in the (a) pre-stent and (b) post-stent geometries of case E1 at systolic peak. Point A and B indicate a splitting flow region and the flow jet entering the aneurysm; Point C indicates a large recirculation flow zone at the aneurysm fundus.	44
Figure 24 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case E1. Maximum and mean OSI on the pre- and post-stent aneurysm surfaces: 0.43 and 0.026 versus 0.38 and 0.013, respectively.	44
Figure 25 – Mesh and time-step independence analysis for the post-stent geometry of case 11: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	57
Figure 26 – Area-averaged WSS on the post-stent surface of case 11 as a function of time for meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.	58
Figure 27 – Mesh and time-step independence analysis for the pre-stent geometry of case 11: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	58
Figure 28 – Area-averaged WSS on the pre-stent surface of case 11 as a function of time for meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.	59
Figure 29 – Mesh and time-step independence analysis for the post-stent geometry of case 16: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	60
Figure 30 – Area-averaged WSS on the post-stent surface of case 16 as a function of time for meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.	60
Figure 31 – Mesh and time-step independence analysis for the pre-stent geometry of case 16: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	61

Figure 32 – Area-averaged WSS on the pre-stent surface of case 16 as a function of time for meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.	61
Figure 33 – Mesh and time-step independence analysis for the post-stent geometry of case 17: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,300,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	62
Figure 34 – Area-averaged WSS on the post-stent surface of case 17 as a function of time for different combinations of mesh and time-step resolution. . .	63
Figure 35 – Mesh and time-step independence analysis for the pre-stent geometry of case 17: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 950,000$, and $\sim 1,300,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	63
Figure 36 – Area-averaged WSS on the pre-stent surface of case 17 as a function of time for different combinations of mesh and time-step resolution. . . .	64
Figure 37 – Mesh and time-step independence analysis for the post-stent geometry of case E1: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	65
Figure 38 – Area-averaged WSS on the post-stent surface of case E1 as a function of time for meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-5} s.	65
Figure 39 – Mesh and time-step independence analysis for the pre-stent geometry of case E1: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.	66
Figure 40 – Area-averaged WSS on the pre-stent surface of case E1 as a function of time for meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-5} s.	66
Figure 41 – Arbitrary polygonal element of a finite volume mesh, and its neighboring elements.	69
Figure 42 – Over-relaxed decomposition of the normal surface vector $\mathbf{s}_f$. $\mathbf{E}_f$ lays in the $\mathbf{d}_{CF}$ direction and $\mathbf{T}_f$ is normal to $\mathbf{s}_f$	73
Figure 43 – Schematic representation of the assembled linear system of algebraic equations: a_C^ϕ coefficients are find at the matrix diagonal and a_F^ϕ coefficients occupy other positions in the line.	76

LIST OF TABLES

Table 1	–	Percentage of ruptured aneurysms based on the aneurysm size and location.	19
Table 2	–	Geometric characteristics of the aneurysms in the current study: parent artery and its diameter d_a , neck diameter d_n , dome height h_d and diameter d_d , aspect ratio A_r , and mean blood flow rate through its parent artery $\bar{q}_a$.	28
Table 3	–	Comparison of maximum and mean values of WSS and OSI on the pre- and post-stent aneurysm surfaces of case 11, case 16, case 17, and case E1.	45
Table 4	–	Summary of the findings of the current work. WSS and OSI values expressing the percent variation after vascular remodeling.	46

LIST OF ABBREVIATIONS

3DRA	Three-dimensional rotational angiography
ACA	Anterior cerebral artery
ACoA	Anterior communicating artery
BA	Basilar artery
CFD	Computational fluid dynamics
CV	Control volume
FIZ	Flow impingement zone
FVM	Finite volume method
ICA	Internal carotid artery
MCA	Middle cerebral artery
OSI	Oscillatory shear index
PISO	Pressure implicit with splitting operators
SACE	Stent-assisted coil embolization
SAH	Subarachnoid hemorrhage
SIMPLE	Semi-implicit method for pressure linked equations
V&V	Validation and verification
VOI	Volume of interest
WSS	Wall shear stress

ETHICS STATEMENT

We hereby declare that, to the best of our knowledge, the current study had no influence on any decisions taken by Dr. Carlos Eduardo Baccin regarding the treatment of the aneurysms presented here.

CONTENTS

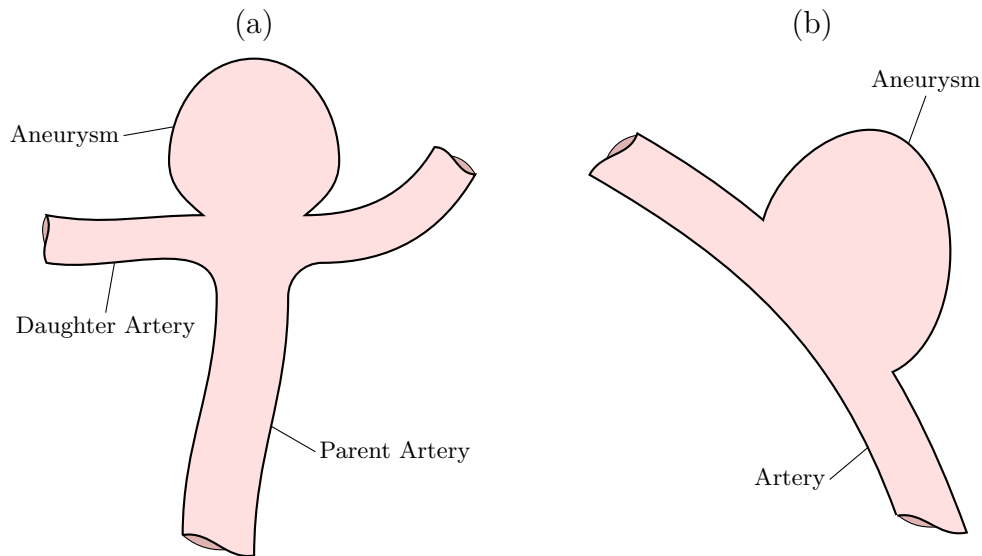
1	INTRODUCTION	17
2	METHODOLOGY	23
2.1	Physical and mathematical modeling	23
2.2	Numerical methods	25
2.2.1	Domain discretization	26
2.2.2	Discretization of the mathematical model	30
2.3	Hardware support	34
2.4	Data analysis	35
3	RESULTS	37
3.1	Case 11	37
3.2	Case 16	39
3.3	Case 17	41
3.4	Case E1	43
4	DISCUSSION AND CONCLUSIONS	46
	REFERENCES	49
	APPENDICES	55
A	MESH AND TIME-STEP INDEPENDENCE STUDY	56
A.1	Case 11	56
A.2	Case 16	59
A.3	Case 17	62
A.4	Case E1	64
A.5	Final considerations	67
B	THE FINITE VOLUME DISCRETIZATION	68
B.1	Spatial discretization	70
B.2	Temporal discretization	74
B.3	Pressure-velocity coupling	77
C	RESIDUALS IN OPENFOAM	82

1 INTRODUCTION

Strokes are the main cause of long-term disabilities and the third cause of death in western countries, only behind heart attack and cancer [1, 2]. It consists of the death of brain tissue by poor oxygen supply as a result of two events: brain ischemia and subarachnoid hemorrhage (SAH). The former is caused by insufficient blood flow to the brain [3]; the latter, on the other hand, by bleeding into the subarachnoid space. It has been estimated that 9 out of 100.000 individuals experience SAH each year in western countries [4], 85% of which are caused by the rupture of intracranial aneurysms [5].

Aneurysms are vascular disorders in which an abnormal balloon arises on the arterial wall (Figure 1). These aneurysms can occur at different locations of the human vascular system, more commonly found on the abdominal aorta and on the arteries that reach the brain. Intracranial aneurysms frequently appear on bifurcations of the circle of Willis [1]—an interconnected circulatory structure that supplies blood to the brain (Figure 2).

Figure 1 – Schematic illustration of (a) bifurcation and (b) sidewall aneurysms.

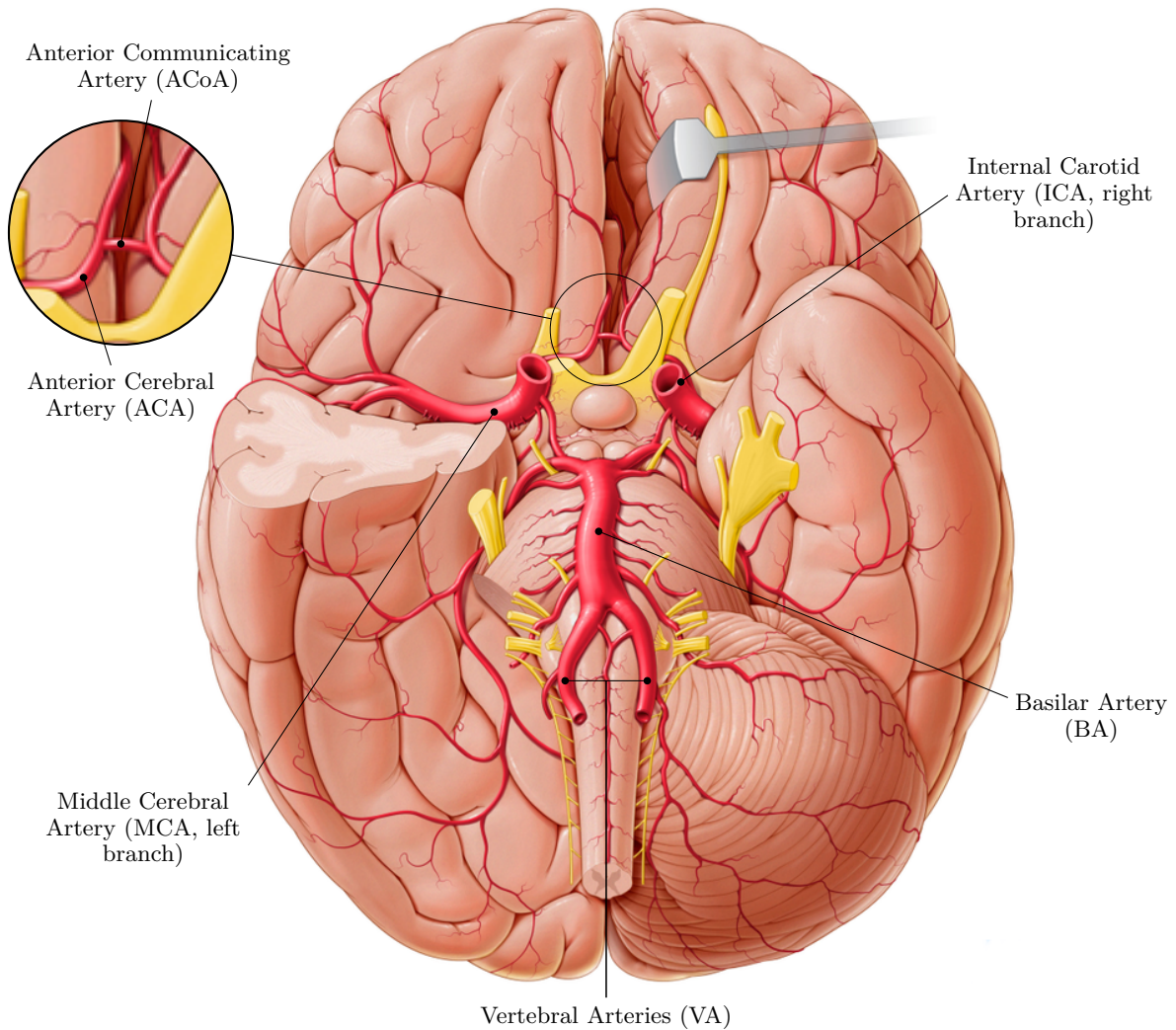


Source: prepared by the author.

Statistics have shown that 2–5% of the population worldwide carry one or more intracranial aneurysms [7, 8], 2% of which will eventually rupture resulting in subarachnoid hemorrhage [9]. Despite the recent improvements in medicine, subarachnoid hemorrhage remains a serious disease with a 50% death rate [10] and a 12–30% long-term or permanent disabilities rate [11].

Aneurysms are usually asymptomatic, making their discovery merely incidental. Recent improvements and availability of non-invasive neuroradiological imaging techniques

Figure 2 – Inferior view of the base of the brain showing an interconnected circulatory structure composing the circle of Willis—internal carotid arteries (ICA) and their branches: middle cerebral arteries (MCA) and anterior communicating arteries (ACA); the vertebrobasilar system, composed of the vertebral arteries (VA) and the basilar artery (BA); and the anterior communicating artery (ACoA), connecting the left and right branches of the ACA.



Source: prepared by the author with brain image extracted from KenHub [6].

have made their discovery more frequent. To date, most physicians rely on statistical correlations to determine risk of aneurysm rupture and viability of preventive treatments. According to Wiebers and Unruptured Intracranial Aneurysms Investigators [12], the risk of rupture increases with the aneurysm size (Table 1).

Along with aneurysm size, aneurysm aspect ratio—dome height/neck width—has been consistently used to evaluate the risk of rupture. According to Weir et al. [13], the risk of rupture is 20-fold greater for aneurysms with an aspect ratio greater than 3.47 compared to those with an aspect ratio lower than 1.38. However, due to the poor prognosis for subarachnoid hemorrhage, physicians often consider preventive treatments when an

Table 1 – Percentage of ruptured aneurysms based on the aneurysm size and location.

Aneurysms location	< 7 mm	7–12 mm	12–24 mm	≥ 25 mm
ACA, MCA, and ICA	0%	2.6%	14.5%	40%
BA and VA	2.5%	14.5%	18.4%	50%

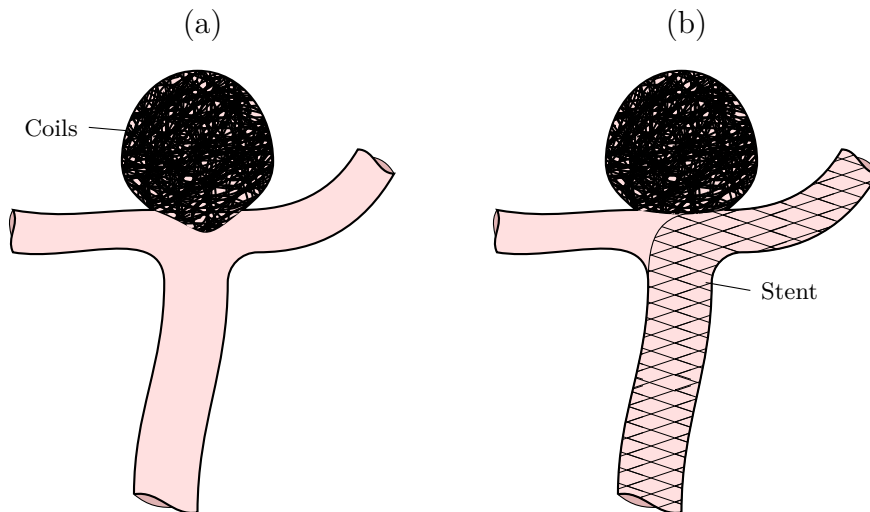
Source: Wiebers and Unruptured Intracranial Aneurysms Investigators [12].

unruptured aneurysm is identified.

Currently, the two leading treatment techniques for intracranial aneurysms are surgical intervention—direct clipping, for example—and endovascular treatment—coils placement inside the aneurysm, assisted or not by stents. According to Qureshi et al. [14], post-procedure disabilities are more frequent in patients who undergo surgery compared to those who undergo endovascular treatments (25% versus 8%); also the number of days in intensive care, the length of stay in hospital, and treatment costs are all greater for surgical interventions. Therefore, many physicians have been considering coils, assisted or not by stents (Figure 3), as a primary option to treat unruptured aneurysms.

Stent-assisted coil embolization (SACE) of intracranial aneurysms was first designed to treat fusiform or wide-neck aneurysms—ratio between aneurysm neck and aneurysm dome height greater than 0.5 or neck size greater than 4 mm—in which other neurovascular treatments were not feasible [15, 16]. However, with gained experience and introduction of specifically-designed self-expanding stents for intracranial use, SACE has been employed to treat a large range of aneurysms [17] in various configurations [18].

Figure 3 – Schematic illustration of coiling techniques: (a) stand-alone coil embolization and (b) stent-assisted coil embolization.



Source: prepared by the author.

Some authors have also proposed using stents as a stand-alone procedure to treat fusiform aneurysms, obtaining gradual aneurysm occlusion [19–22]. The authors speculate that stand-alone stents could create favorable thrombogenic conditions by altering intracranial blood flow (hemodynamics), which has been related to aneurysm initiation, development and rupture [23–25].

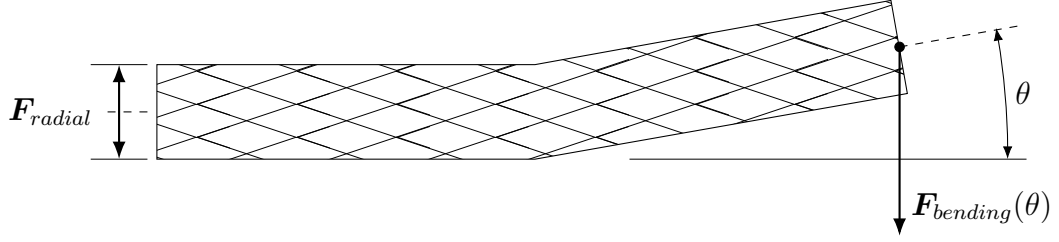
Out of the various hemodynamic parameters, the wall shear stress (WSS) due to the flow velocity gradient adjacent to the aneurysm wall has been reported to play a major role in the different stages of aneurysm growth [23, 26]. In the human arterial system, high WSS levels can trigger biological mechanisms associated with arterial remodeling, leading to initiation, development, and rupture of aneurysms [24]. On the other hand, it has also been advocated that low WSS have a negative effect on endothelial cells, being an important contributor to aneurysm growth and rupture [23, 27]. Towards an unifying hypothesis, Meng et al. [25] took a step further and proposed that both high and low WSS can drive aneurysm growth and rupture. According to the authors, a combination of low WSS and elevated oscillatory shear index (OSI)—a parameter that measures the changes in the WSS vector direction within a cardiac cycle—triggers a destructive pathway associated with growth and rupture of large aneurysms; whereas a combination of high WSS and positive spatial WSS gradient along the flow triggers a destructive pathway associated with growth of small or secondary bleb aneurysm.

In light of the role exerted by hemodynamics in the different stages of aneurysm development, experimental and numerical studies have been conducted to investigate hemodynamic changes induced by stents [4, 9, 18, 28–33]. Cantón et al. [28] measured changes in flow dynamics using digital particle image velocimetry in flexible silicone sidewall aneurysms models after sequential stent placement and concluded that the velocity magnitude of the flow jet entering the aneurysm could be reduced by more than 50%.

Tang et al. [29] performed numerical simulations of a bifurcation aneurysm to evaluate the influence of the aneurysm neck size after stenting and concluded that the maximum velocity inside the aneurysm at systolic phase was reduced by 18–24%; and that the volume flow rate entering the aneurysm over the entire cardiac cycle could be reduced by more than 50%. Bernardini et al. [9] performed numerical simulations of a idealized sidewall aneurysm for two stent positions and arrived at similar conclusions to those of Cantón et al. [28] and Tang et al. [29]. To date, we note that most of the studies have been focusing on the hemodynamic changes caused by the presence of the stent itself, i.e., the blockage effect exerted by the struts.

The current generation of self-expanding intracranial stents are made of shape-memory nickel-titanium alloy (nitinol), granting flexibility and conformability in tortuous vessels. These stents exert a continuous outward-directed radial force and, in addition, a mild force in resisting bending motion [34] (Figure 4). The former is necessary to maintain

Figure 4 – Schematic illustration of a shape-memory alloy stent subject to a bending angle θ . $\mathbf{F}_{bending}$ is a resulting counteracting force dependent on θ and $\mathbf{F}_{radial}$ is an ever-present outward-directed radial force as a result of the self-expanding design of the stent.



Source: prepared by the author.

a firm grip on the vessel wall; the latter is a secondary, collateral effect that has been related to immediate and delayed angular remodeling of the local vascular system [18, 35, 36].

Gao et al. [37] evaluated the immediate and delayed stent-induced vascular remodeling for bifurcation aneurysms at different arteries of the brain. The authors reported an immediate variation of 20° in the bifurcation angle; further variations were observed in up to one year follow-ups with a total angular change of 35° . According to the authors, the greatest changes were observed within 6 months posttreatment, followed by minor changes until one year follow-up, suggesting an asymptotic behavior. Furthermore, the authors reported the angular remodeling being inversely proportional to the parent artery diameter and proportional to the pretreatment angle; i.e., the smaller the parent vessel or the prestenting vascular angle, the bigger the posttreatment angular modification.

More recently, Kono, Shintani, and Terada [38] compared the influence of angular remodeling against the blockage effect of stent struts for sidewall aneurysms. The authors concluded that the stent struts have approximately twice as strong effect on reduction of flow velocity than angular remodeling. Jeong, Han, and Rhee [39] performed a similar study for a group of idealized bifurcation aneurysms, adopting a porous-medium methodology to represent the coils inside the aneurysm sac. According to the authors, angular remodeling may provide an unfavorable hemodynamic environment, which might delay thrombus formation.

Despite the valuable contributions of the above-mentioned studies, we still lack information regarding hemodynamic changes caused by stent-induced vascular remodeling in bifurcation aneurysms without the presence of coils. This is of particular interest to stand-alone stent treatment [19–22]; and also to two-step stent-assisted coiling technique [40], in which stenting and coiling are done in separate steps.

Objectives

Using patient-specific models of bifurcation intracranial aneurysms before and after vascular remodeling, we propose to use results of numerical simulations to evaluate the changes in hemodynamic parameters related to aneurysm growth and rupture—WSS and OSI—according to reference values found in the literature and determine whether endovascular treatments could benefit from stent-induced vascular remodeling. Furthermore, we use only open-source tools during all stages of the current work, making our methodology easily available.

2 METHODOLOGY

Blood flow in aneurysms and arteries may be modeled and solved in different ways. As presented in Chapter 1, we propose to solve this problem numerically, making use of the Finite Volume Method (FVM) [41–43]. Thus, we present throughout this chapter the methodology behind our study: physical modeling, boundary conditions, discretization of the governing equations by the FVM, reconstruction of patient-specific aneurysm geometries from medical images, and data analysis strategy.

2.1 Physical and mathematical modeling

Before we present the physical and mathematical modeling, we must define a group of hypothesis. In the literature, hypothesis of rigid vessel walls and blood as an incompressible Newtonian fluid in a isothermal, laminar flow regime are commonly adopted to study blood flow in aneurysms and arteries [2, 7, 33, 44].

Different studies already evaluated the influence of these hypothesis on hemodynamic parameters, such as velocity field and WSS distribution on the arterial wall [26, 45–49]. In general, they have a much lower influence on hemodynamics than changes in the geometry of aneurysms and arteries [45]—the exact subject of this study. Thereby, we adopt the same group of hypothesis in our study, considering a blood density of $1,000 \text{ kg/m}^3$ and a kinematic viscosity of $3.3 \times 10^{-6} \text{ m}^2/\text{s}$ [50].

In this case, we face a classical problem of fluid dynamics, in which the governing equations are derived from the principle of conservation of mass and the balance of linear momentum, respectively, as follows:

$$\nabla \cdot (\rho \mathbf{v}) = 0, \quad (2.1)$$

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{f}_b, \quad (2.2)$$

where $\mathbf{v}$ and p are the flow velocity field and the pressure field, respectively; ρ is the blood density; $\mathbf{f}_b$ represents the body forces field per volume; and $\boldsymbol{\tau}$ is the stress tensor, which can be expressed as follows for a Newtonian fluid with constant properties:

$$\boldsymbol{\tau} = \mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T] - \frac{2}{3} \mu (\nabla \cdot \mathbf{v}) \mathbf{I} \xrightarrow[\mu = \text{constant}]{\rho = \text{constant}} \boldsymbol{\tau} = \mu \nabla^2 \mathbf{v}, \quad (2.3)$$

where μ is the blood dynamic viscosity and $\mathbf{I}$ is the second rank identity tensor. Moreover, it will be useful for us to express the governing equations in their integral form, which is of special interest to the finite volume method. Therefore, Equations 2.1 and 2.2 can be

written as

$$\oint_S \rho \mathbf{v} \cdot \mathbf{n} \, dS = 0 \quad (2.4)$$

and

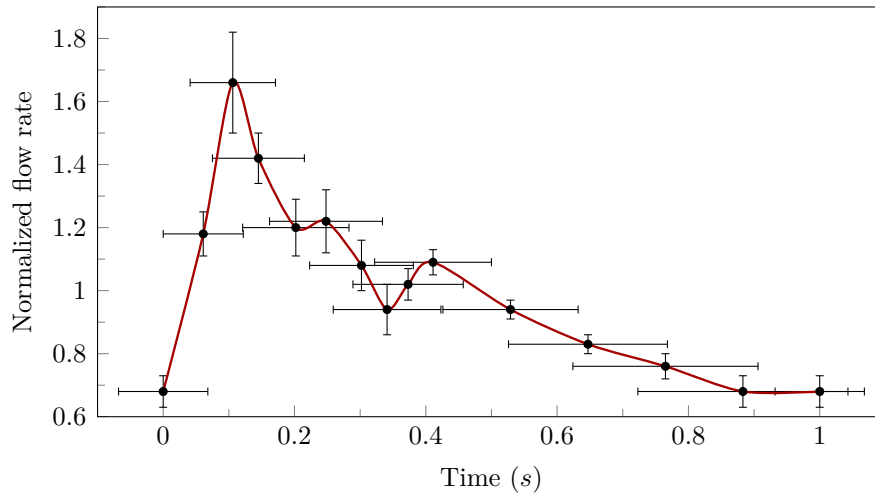
$$\frac{\partial}{\partial t} \int_V \rho \mathbf{v} \, dV + \oint_S \rho \mathbf{v} (\mathbf{v} \cdot \mathbf{n}) \, dS = - \oint_S p \mathbf{n} \, dS + \oint_S \mu \nabla \mathbf{v} \cdot \mathbf{n} \, dS, \quad (2.5)$$

where $\mathbf{n}$ is the unit normal vector to S pointing outward.

In Equations 2.4 and 2.5, we identify the flow velocity and pressure field as the unknowns, both as functions of the spatial coordinates and the time. Therefore, we must define appropriate initial and boundary conditions.

At the inlet—the cross section in the aneurysm parent artery—we impose a zero pressure gradient and a time-varying velocity, corresponding to the flow pulse from the beginning of systole until the end of the diastole. The aneurysms in the current study are located in different bifurcations of the cerebral vascular system. Since we do not have patient-specific information on the blood flow rate profile in the aneurysm parent artery, we used available data in the literature to obtain the inlet flow velocity for each case. For that, we first considered a pulsatile normalized blood flow, as shown in Figure 5. Ford et al. [51] measured this profile in the internal carotid artery (ICA) and normalized it with respect to the temporal mean blood flow rate in the same artery. Then, to obtain the dimensional profile we multiplied the normalized profile by the mean blood flow rate in the artery of interest. The mean blood flow rate for different arteries of the cerebral vascular system is provided by Zarrinkoob et al. [52]. The authors measured it as a percentage of

Figure 5 – Blood flow rate for the internal carotid artery (ICA) normalized with respect to the temporal mean blood flow rate.



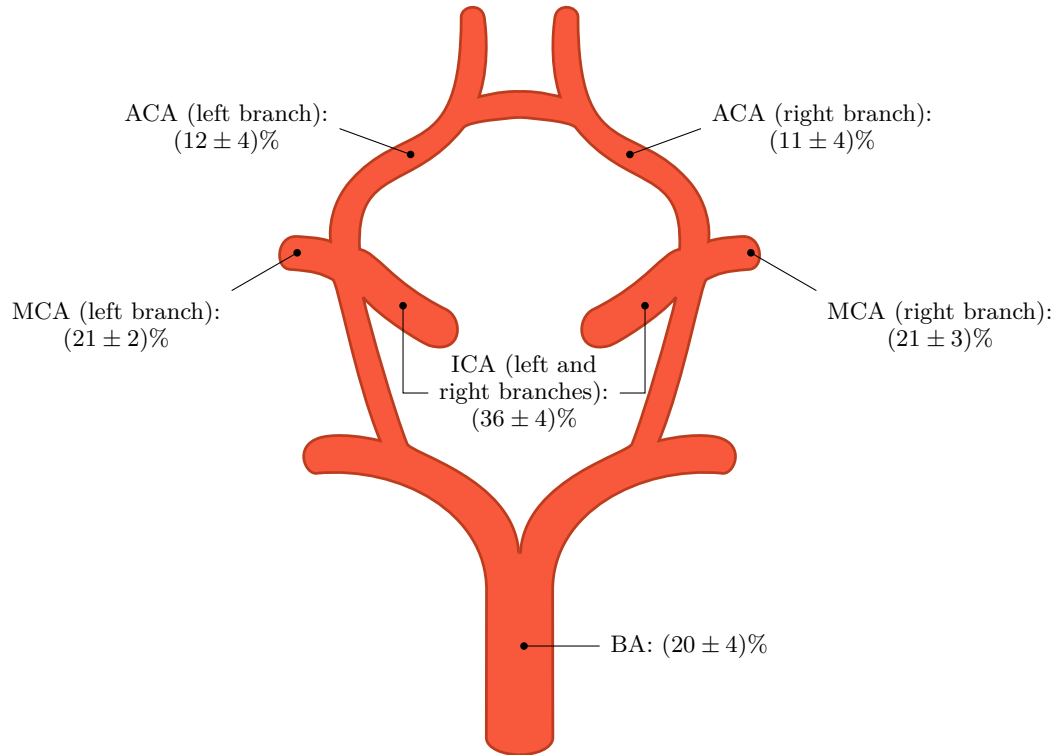
Source: prepared by the author with experimental data from Ford et al. [51].

the total blood flow rate to the brain in normal subjects, which is (11.95 ± 2.05) ml/s, as shown in Figure 6. Finally, we computed the inlet flow velocity using the cross sectional area of the inlet boundary.

At the outlet—the cross section in the daughter arteries of the vessel bifurcation—we imposed a fixed pressure condition and a zero velocity gradient. Note that for incompressible flows, the pressure field is computed relative to a reference value and commonly set to zero by default. Nevertheless, we adopted a constant pressure equal to the average pressure level in the human body, approximate 100 mmHg or 13.33 Pa.

Lastly, at vessel walls we imposed a no-slip condition, assuming a zero relative velocity between flow and vessel walls.

Figure 6 – Mean blood flow rate through the arteries of the brain as a percentage of the total blood flow rate reaching the brain: (11.95 ± 2.05) ml/s.



Source: prepared by the author with data from Zarrinkoob et al. [52].

2.2 Numerical methods

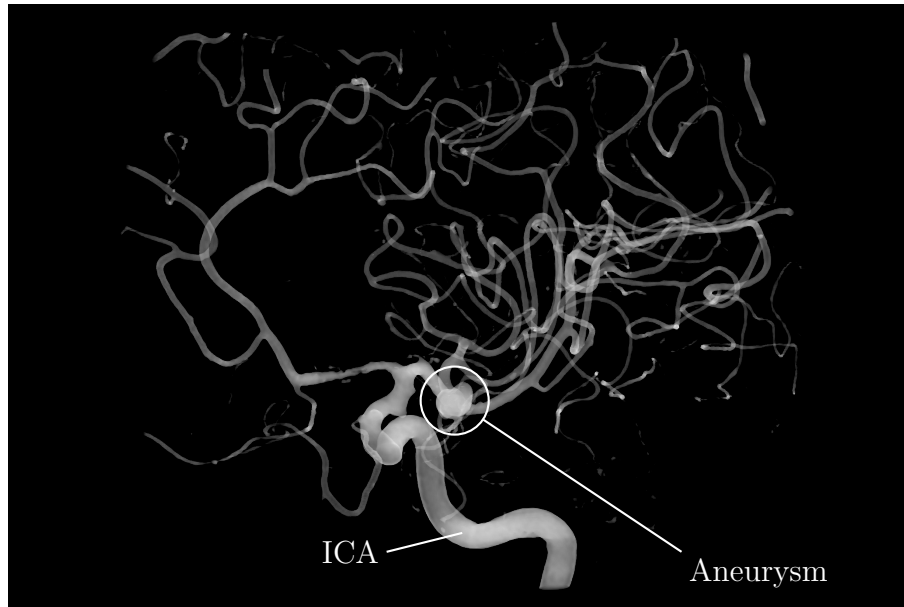
To solve the governing equations—Equations 2.1 and 2.2—under the boundary conditions presented in Section 2.1 we chose the Finite Volume Method [41, 43]. We used the software OpenFOAM (Open-source Field Operation and Manipulation) [53, 54], which is the leading free, open-source software for Computational Fluid Dynamics (CFD). In this section we present the domain discretization procedure followed by the discretization procedure of the governing equations.

2.2.1 Domain discretization

The domain discretization was performed splitting the geometry into a finite number of 3D uniform elements, also known as control volumes. To this end, we first needed to obtain the geometry of the aneurysm and surrounding arteries. Geometries of aneurysms were obtained from images of 3D rotational angiography (3DRA). These images were taken using a Philips Allura Xper FD20 and provided by Dr. Carlos Eduardo Baccin (Hospital Israelita Albert Einstein, São Paulo, Brazil).

The 3DRA file is a 3D pixelized image that provides a clear visualization of the cerebral vascular system—see Figure 7—and thus used by many interventional neuroradiologists. To reconstruct the aneurysm geometry from the 3DRA file, we performed the following steps using the Vascular Modeling Toolkit (VMTK), an open-source collection of libraries and tools for 3D reconstruction, geometric analysis, mesh generation, and surface data analysis for image-based modeling of blood vessels.

Figure 7 – Volume rendering representation of a 3DRA image file. Picture taken using the visualization software ParaView.

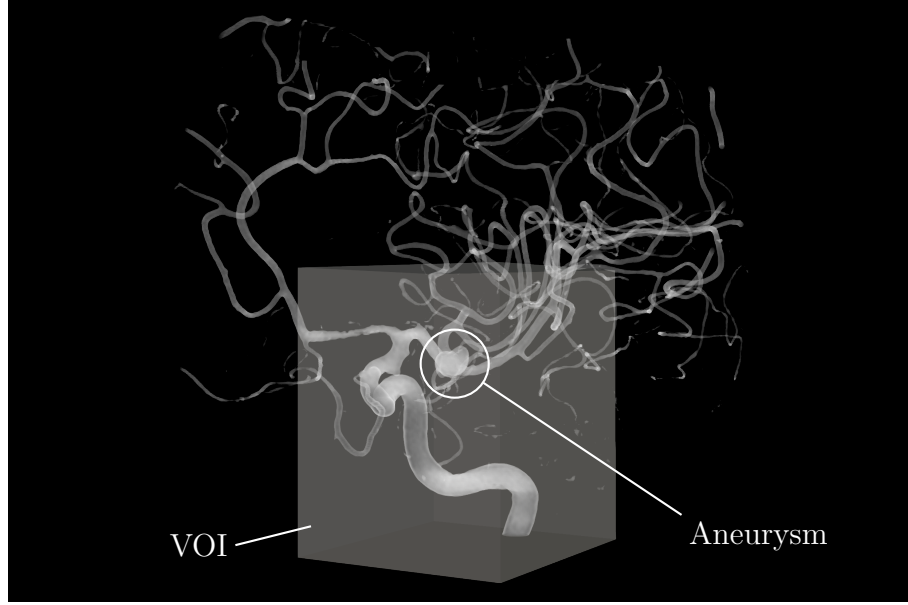


Source: prepared by the author.

First, we selected a volume of interest (VOI), a small portion of the 3DRA image that encloses the aneurysm and its closest vessels, as shown in Figure 8. For that, VMTK provides an utility called `vmtkimagevoiselector`. This utility extracts the VOI from the 3DRA image and saves it in a separate image file, enabling us to load just the VOI image file during future steps of the reconstruction procedure.

Second, to reconstruct the surface of the aneurysm and surrounding vessels inside the VOI we used two utilities: `vmtklevelsetsegmentation` and `vmtkmarchingcubes`. The former uses a series of filters and user-defined thresholds to create an initial level set and

Figure 8 – Volume rendering representation of a 3DRA image file. Volume of interest (VOI) enclosing the aneurysm and its surrounding vessels. Picture taken using the visualization software ParaView.



Source: prepared by the author.

evolve it to image gradients; the latter uses these image gradients to generate a triangulated isosurface.

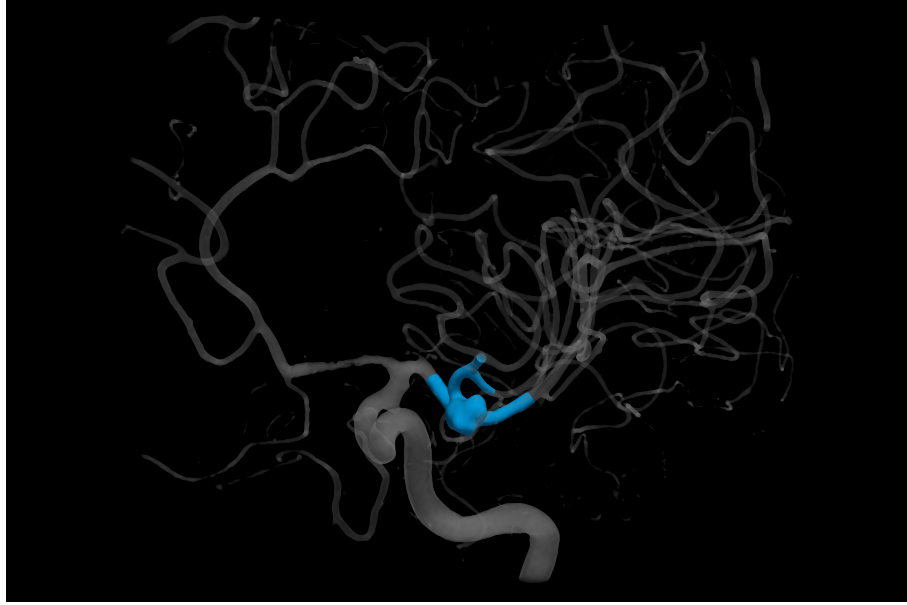
Normally the isosurface generated does not have a production-ready surface quality. Therefore, as a third step, we used two utilities to increase the surface quality: `vmtksurfaceremeshing` and `vmtksurfacesmoothing`. Remeshing the surface, increases the number of triangulated elements, thereby, improving the efficiency of the smoothing algorithms used by VMTK.

Lastly, we used the utility `vmtksurfaceclipper` to create inlet and outlet boundaries, clipping the surrounding arteries of the aneurysms, and then yielding the final aneurysm surface. We used this surface to determine the geometric parameters of the aneurysm and its surrounding arteries.

Table 2 provides the following parameters of the cases in the current study: aneurysm height h_d , neck diameter d_n , parent artery name, aneurysm aspect ratio—defined as h_d/d_n —and mean blood flow rate in the parent artery $\bar{q}_a$ —as defined in Section 2.1. We kept the nomenclature of the original 3DRA files as case identifiers. The reconstructed surfaces of each case are presented in Figure 10.

Finally, meshes were created from the above-mentioned surface using the utility `vmtkmeshgenerator`. This utility has numerous options to control mesh quality and size, creating a volume filled with tetrahedral elements in the core and prismatic elements adjacent to the vessel wall.

Figure 9 – Volume rendering representation of a 3DRA image; blue surface highlights the final aneurysm surface reconstructed using VMTK utilities. Picture taken using the visualization software ParaView.



Source: prepared by the author.

Table 2 – Geometric characteristics of the aneurysms in the current study: parent artery and its diameter d_a , neck diameter d_n , dome height h_d and diameter d_d , aspect ratio A_r , and mean blood flow rate through its parent artery $\bar{q}_a$.

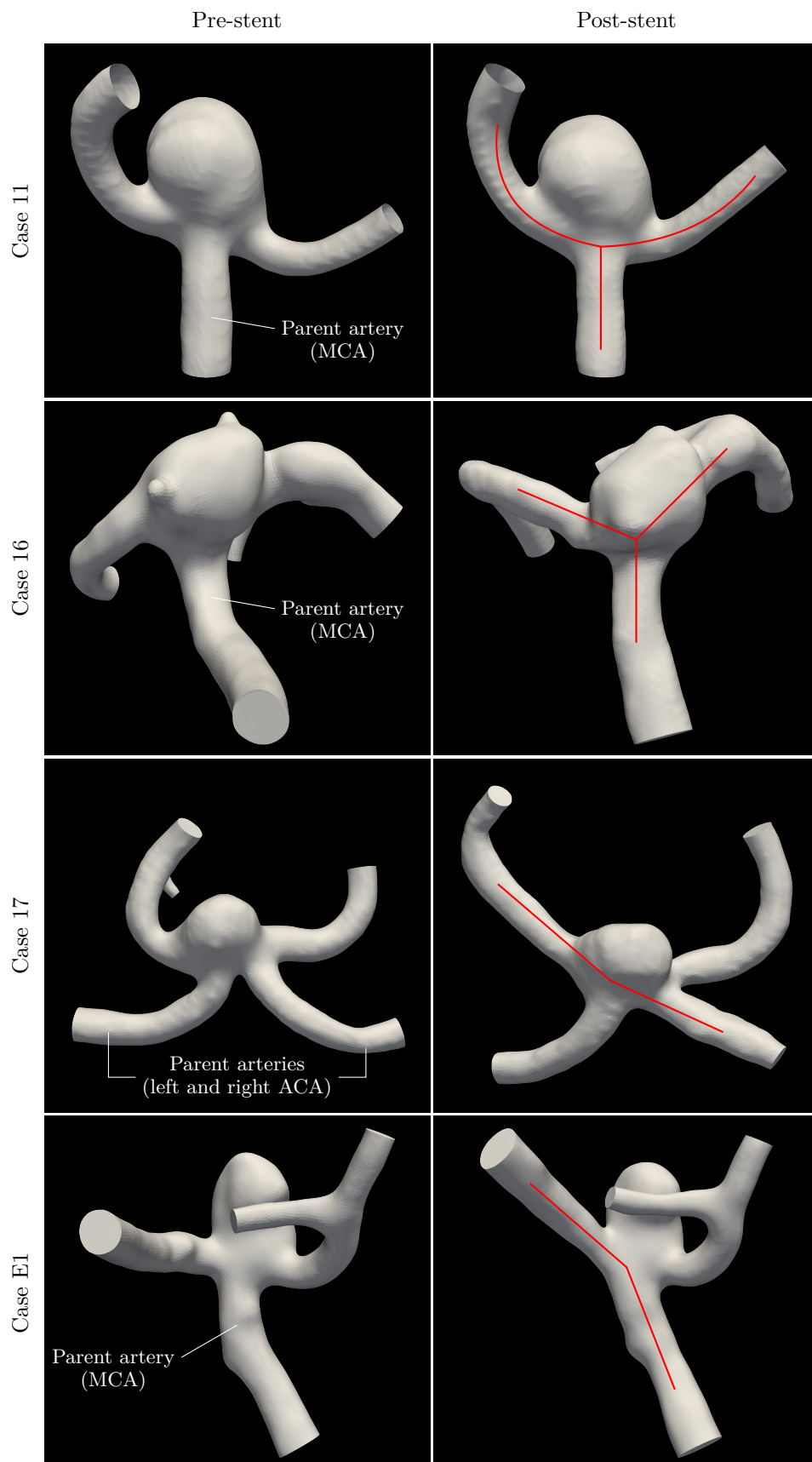
		Parent artery	d_a (mm)	d_n (mm)	h_d (mm)	d_d (mm)	A_r	$\bar{q}_a$ (ml/s)
Case 11	pre-stent	MCA	2.7	7.0	8.7	9.6	1.25	2.5
	post-stent		2.7	7.4	8.7	9.6	1.17	
	% variation		0%	+5.7%	0%	0%	-6.4%	
Case 16	pre-stent	MCA	2.5	6.5	5.4	6.4	1.20	2.5
	post-stent		2.9	5.7	5.6	6.0	1.01	
	% variation		+16%	-12.3%	+3.7%	-6.3%	-15.8%	
Case 17	pre-stent	ACA	2.3 & 2.1*	5.9	5.0	5.1	1.18	1.4 [†]
	post-stent	(both branches)	1.9 & 1.7*	5.6	4.5	4.7	1.24	
	% variation		-17.4% & -19%*	-5.1%	-10%	-7.8%	+5.1%	
Case E1	pre-stent	MCA	3.3	4.5	5.7	5.9	1.27	2.5
	post-stent		3.7	5.1	4.8	5.7	0.94	
	% variation		+12.1%	+13.3%	-15.8%	-3.4%	-26%	

* left & right ACA

[†] per branch

Source: prepared by the author.

Figure 10 – Reconstructed surfaces of case 11, case 16, case 17, and case E1. Red lines illustrate where stents were deployed.

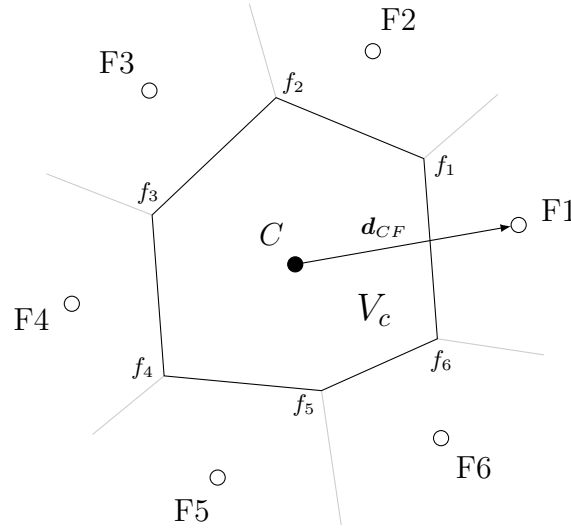


Source: prepared by the author.

2.2.2 Discretization of the mathematical model

Coded in C++, OpenFOAM combines utilities for pre- and post-processing, and solvers for partial differential equations, offering a complete framework for solving problems of Continuum Mechanics. OpenFOAM uses the FVM with cell-centered variable arrangement, i.e., unknown quantities are stored at cell centroids. A typical finite-volume mesh is composed of non-overlapping, arbitrary polygonal elements with flat faces, as shown in Figure 11. Moreover, each face must be shared by only two neighboring cells; exceptions are those composing the boundaries of the domain, which in turn belong to only one cell. All meshes used in this study follow these conditions.

Figure 11 – Arbitrary polygonal control volume V_C with centroid C of a 2D finite volume mesh, and its neighboring cells with centroid F_i .



Source: prepared by the author.

The finite volume discretization procedure is initiated by writing the governing equations as integrals over a control volume V_C . Then, Gauss' divergence theorem is used to transform the volume integrals of the advective and diffusive terms into sums of surface integrals over control volume faces. To evaluate the face integrals, we assume the fields to behave linearly around control volume centroids; thus, using an one-point Gaussian quadrature yields a second-order accurate spatial discretization. The whole procedure is detailed in Appendix B and deeply grounded on the writings of Versteeg and Malalasekera [41], Ferziger and Peric [42], and Moukalled, Mangani, and Darwish [43]. Our main focus here is to apply this procedure to the governing equations: Equations 2.4 and 2.5.

The semi-discretized momentum equation for a control volume V_C in a finite volume

mesh is expressed as

$$\rho V_C \frac{3\mathbf{v}_C^n - 4\mathbf{v}_C^{n-1} + \mathbf{v}_C^{n-2}}{2\Delta t} + \sum_{f \sim \text{nb}(C)} (\dot{m}_f \mathbf{v}_f^n) = \sum_{f \sim \text{nb}(C)} [\mu(\nabla \mathbf{v})_f^n \cdot \mathbf{s}_f] + (\nabla p)_C^n V_C, \quad (2.6)$$

where $f \sim \text{nb}(C)$ denotes faces neighboring centroid C — see Figure 11; the subscripts f and C indicate values evaluated at face centroid and control volume centroid, respectively; the superscript n represents the time-step level; $\mathbf{s}_f$ is a vector with magnitude equal to the face area, normal to face f , and pointing outwards control volume V_C ; $\dot{m}_f = \rho(\mathbf{v}_f \cdot \mathbf{s}_f)$ is the mass flow rate through face f and thus, must satisfy the discretized principle of conservation of mass:

$$\sum_{f \sim \text{nb}(C)} \dot{m}_f = \sum_{f \sim \text{nb}(C)} \rho(\mathbf{v}_f \cdot \mathbf{s}_f) = 0. \quad (2.7)$$

Note that because we evaluate the mass flow rate $\dot{m}_f$ using known values from the previous iteration, we use no superscript to denote time-step level.

To evaluate face values in Equation 2.6, we interpolate values at cell centroids. For the velocity in the advective term, $\mathbf{v}_f^n$, we adopt a second-order Upwind scheme for unstructured grids, which yields

$$\mathbf{v}_f = \mathbf{v}_C + [2(\nabla \mathbf{v})_C - (\nabla \mathbf{v})_f] \cdot \mathbf{d}_{Cf}, \quad (2.8)$$

where $\mathbf{d}_{Cf}$ is the vector joining centroid C and face f . Using the least-square method [43] to discretize the velocity in Equation 2.8 yields

$$\mathbf{v}_f = w\mathbf{v}_C + (1 - w)\mathbf{v}_F, \quad (2.9)$$

where the subscript F represents a cell centroid, whose face f is shared with element C ; and w is a weight factor that depends on the chosen interpolation scheme and accounts for the influence of $\mathbf{v}_C$ and $\mathbf{v}_F$ on $\mathbf{v}_f$.

To interpolate the gradient normal to face f in Equation 2.6, $(\nabla \mathbf{v})_f \cdot \mathbf{s}_f$, we used a non-orthogonal corrected scheme as follows:

$$(\nabla \mathbf{v})_f \cdot \mathbf{s}_f = \underbrace{(\nabla \mathbf{v})_f \cdot \mathbf{E}_f}_{\text{orthogonal contribution}} + \underbrace{(\nabla \mathbf{v})_f \cdot \mathbf{T}_f}_{\text{non-orthogonal contribution}}, \quad (2.10)$$

where $\mathbf{s}_f = \mathbf{E}_f + \mathbf{T}_f$, with $\mathbf{E}_f$ being in the direction $\mathbf{d}_{CF}$ —see Figure 11. Thus, Equation 2.10 can be rewritten as

$$(\nabla \mathbf{v})_f \cdot \mathbf{s}_f = E_f \frac{\mathbf{v}_F - \mathbf{v}_C}{d_{CF}} + (\nabla \mathbf{v})_f \cdot \mathbf{T}_f, \quad (2.11)$$

where the non-orthogonal contribution, $(\nabla \mathbf{v})_f \cdot \mathbf{T}_f$, is evaluated using an over-relaxed approach—see Appendix B, Section B.1 for more details.

Combining Equations 2.6, 2.9 and 2.10, we can write an algebraic momentum equation for one control volume in a finite volume mesh as follows:

$$a_C^v \mathbf{v}_C^n + \sum_{F \sim \text{NB}(C)} a_F^v \mathbf{v}_F^n = \mathbf{b}_C^v - (\nabla p)_C V_C, \quad (2.12)$$

where a_C^v , a_F^v , and $\mathbf{b}_C^v$ are functions of the flow velocity. Thus, considering all control volumes in a finite volume mesh, we can assemble a system of algebraic linearized equations, yielding

$$\mathbf{A}^v \mathbf{v}^n = \mathbf{b}^v - V_C (\nabla p)_C, \quad (2.13)$$

where $\mathbf{A}$ is the matrix of coefficients a_C and a_F , $\mathbf{v}$ is the velocity solution vector, $\mathbf{b}$ is the vector of source terms, and ∇p is the vector obtained from the discretization of the pressure gradient.

It is important to note that pressure does not appear as a primary variable in either the momentum or continuity equations; furthermore, for incompressible flows, no explicit equation is available to compute the pressure field in the momentum equation, requiring a special treatment for the pressure-velocity coupling. One approach consists of reformulating the governing equations in terms of a momentum and a pressure equation [43], where the pressure equation is a combination of the semi-discretized momentum and continuity equations.

To produce the pressure equation, we start considering the discretized continuity equation, Equation 2.7. Then, we evaluate the flow velocity at face centroids from cell centroids values, using the discretized momentum equation, Equation 2.13, which can be rewritten as

$$\mathbf{v}_C + \mathbf{H}_C[\mathbf{v}] = \mathbf{B}_C^v - \mathbf{D}_C^v (\nabla p)_C, \quad (2.14)$$

where

$$\mathbf{H}_C[\mathbf{v}] = \sum_{F \sim \text{NB}(C)} \frac{a_F^v}{a_C^v} \mathbf{v}_F, \quad \mathbf{B}_C^v = \frac{\mathbf{b}_C^v}{a_C^v}, \quad \text{and} \quad \mathbf{D}_C^v = \frac{V_C}{a_C^v}.$$

However, interpolating flow velocities from cell centroids to face centroids using a linear scheme originates the checkboard problem. A solution to this problem was first proposed by Rhie and Chow [55], where a pseudo-momentum equation is constructed at face centroid. For that, the coefficients of the pseudo-momentum equation are linearly

interpolated from coefficients of momentum equations at cell centroid, yielding

$$\mathbf{v}_f + \mathbf{H}_f[\mathbf{v}] = \mathbf{B}_f^v - \mathbf{D}_f^v(\nabla p)_f \quad (2.15)$$

or

$$\mathbf{v}_f = -\mathbf{H}_f[\mathbf{v}] + \mathbf{B}_f^v - \mathbf{D}_f^v(\nabla p)_f. \quad (2.16)$$

Finally, substituting Equation 2.16 into Equation 2.7, we obtain

$$\sum_{f \sim \text{nb}(C)} \mathbf{D}_f^v(\nabla p)_f \cdot \mathbf{s}_f = \sum_{f \sim \text{nb}(C)} \left\{ \mathbf{B}_f^v - \mathbf{H}_f[\mathbf{v}] \right\} \cdot \mathbf{s}_f, \quad (2.17)$$

where the gradient $(\nabla p)_f \cdot \mathbf{s}_f$ is evaluated implicitly using a non-orthogonal-corrected approach—Equation 2.9, more details in Appendix B, Section B.3. After some algebraic manipulations, we are now able to express a linearized algebraic equation for the pressure

$$a_C^p p_C^n + \sum_{F \sim \text{NB}(C)} a_F^p p_F^n = b_C^p, \quad (2.18)$$

which represents the discretized pressure equation for one finite control volume V_C . Thus, assembling for the whole finite volume mesh, we obtain a linearized system of equations

$$\mathbf{A}^p \mathbf{p}^n = \mathbf{b}^p. \quad (2.19)$$

To handle the solution of the governing equations, as well as the pressure-velocity coupling, we adopted the PISO (Pressure-Implicit Split Operators) algorithm [56]. The algorithm first sets the boundary and initial conditions for the velocity and pressure fields. Next, it solves the discretized momentum equation – Equation 2.13 – yielding an intermediate velocity field, which does not necessarily satisfies the continuity. Then, the intermediate velocity field is used to solve the pressure equation – Equation 2.19 – yielding a pressure field that satisfies both the continuity and momentum equations. Lastly, the velocity field is updated using the new pressure field, resulting in a continuity-satisfying velocity field. According to Issa, Gosman, and Watkins [56], two iterations over the pressure equation are able to provide acceptable accuracy.

The system of equations presented in Equation 2.13 is solved using a preconditioned bi-conjugated gradient solver for asymmetric matrices, with a diagonal incomplete Cholesky preconditioner for asymmetric matrices and convergence criterion based on a scaled normalized residual tolerance equal to 1×10^{-6} . For the pressure system, Equation 2.19, we used a geometric agglomerated algebraic multigrid solver, with scaled normalized residual tolerance equal to 1×10^{-6} . For more details on how OpenFOAM calculates the residuals, see Appendix C.

2.3 Hardware support

In many CFD problems, the solution sequence is very time consuming for a single machine running in serial mode. Considering this, OpenFOAM offers an option to run simulations in parallel on distributed processors. Taking advantage of this feature, all simulations were performed in parallel on the following clusters:

- **GridUNESP:** the computational resource of São Paulo State University (UNESP) runs CentOS 6.9 and has a computational structure of:
 - 256 nodes and 2,048 CPU cores (Intel Xeon 2.83 GHz);
 - 4,096 GB of RAM memory (2 GB per core);
 - InfiniBand interconnection 4X DDR (20 Gbps).
- **Cedar:** integrated into the resources of Compute Canada clusters, it is a heterogeneous cluster suitable for a variety of workloads. The cluster runs CentOS 7.4 and has a computational structure of:
 - 1,396 nodes and 58,416 CPU cores (Intel Broadwell E5-2650, Intel Broadwell E5-2683, and Intel Skylake Platinum 8160F);
 - up to 128 GB of RAM memory per node;
 - Intel OmniPath interconnection (100 Gbps).
- **Graham:** it is also integrated into the resources of Compute Canada clusters. The cluster runs CentOS 7.4 on a computational structure of:
 - 1,107 nodes and 35,527 CPU cores (Intel Broadwell E5-2683 and Intel Broadwell E7-4850);
 - up to 128 GB of RAM memory per node;
 - Mellanox FDR (56 Gbps) and EDR (100 Gbps) InfiniBand interconnection.

Note that all clusters were used separately.

OpenFOAM uses a parallel computing method known as domain decomposition, i.e., it breaks the geometry and associated fields into smaller pieces and allocates them to separate processors for solution. For this task, we used a built-in decomposition method known as Scotch. This method attempts to minimize the number of processor boundaries, reducing the amount of data shared between processors.

Despite the capability of the clusters, increasing the number of processors does not necessarily mean a reduction in simulation time. Different factors can slow down the process and act as a bottleneck, these include fractions of code that cannot be parallelized and hardware limitations. Therefore, the number of processors were estimated via simulation

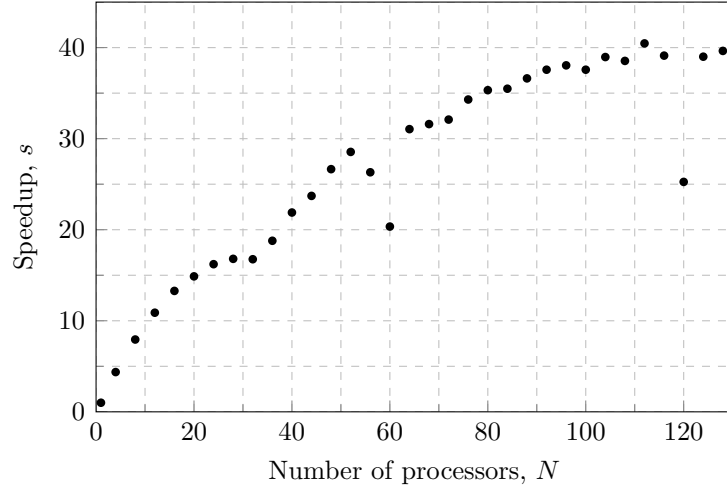
speedup, which measures if a given problem can be solved faster by increasing the number of processors dedicated to that task. The speedup is defined as

$$s = \frac{T_{serial}}{T_{parallel}}, \quad (2.20)$$

where s is the simulations speedup, T_{serial} is the time spent to conclude a task running on a single processor and $T_{parallel}$ is the time spent to conclude the same task running on N processors.

Figure 12 shows the speedup measured for the pre-stent geometry of case 11. Note that, despite the fluctuations in the speedup value, it increases rapidly in the beginning until reach a plateau after 100 processors.

Figure 12 – Speedup, s , as a function of the number of processors, N , for the pre-stent geometry of case 11.



Source: prepared by the author.

Based on these data, a choice of 104 processors would be reasonable. However, all clusters we used operate on a batch scheduling system with dynamic algorithms to support fair-share access to its resources, i.e., the more processors we ask for, the longer the simulation remains in queue; in the end the simulation may take longer to complete. Therefore, we based our decisions regarding the number of processors on empirical knowledge of the fair-share system. The criterion adopted was 32 cores for meshes smaller than 1,000,000 control volumes and 64 cores for meshes greater than that. In both cases, the average wall clock time spent per simulation was around 18 hours.

2.4 Data analysis

Once completed the simulations, we evaluated the following quantities using ParaView, an open-source, multi-platform data analysis and visualization application:

- Velocity field: to determine flow pattern and impact zone;
- WSS on the wall: the WSS is the shear component of the traction due to the stress tensor, $\boldsymbol{\tau}$, of the flow on the wall:

$$WSS = \|\mathbf{WSS}\|_2 = \left\| \underbrace{\mathbf{n} \cdot \boldsymbol{\tau}}_{\text{total traction}} - \underbrace{[(\mathbf{n} \cdot \boldsymbol{\tau}) \cdot \mathbf{n}] \mathbf{n}}_{\text{traction normal component}} \right\|_2, \quad (2.21)$$

where $\mathbf{n}$ is the unit vector, pointing inwards, normal to the wall surface;

- OSI: this index measures changes in the WSS vector direction during the cardiac cycle and it is defined as

$$OSI = \frac{1}{2} \left(1 - \frac{\left\| \int_0^T (\mathbf{WSS}) dt \right\|}{\int_0^T \|\mathbf{WSS}\|_2 dt} \right), \quad (2.22)$$

where T is the cardiac cycle duration.

These are the most common hemodynamic parameters related to intracranial aneurysms rupture, as presented in Chapter 1. Besides the above-mentioned parameters we also computed the mean value of both WSS and OSI on the aneurysm surface in order to quantify the hemodynamic changes due to vascular remodeling. These are defined as

$$\overline{WSS}_a = \frac{1}{A_a} \left\| \int_S (\mathbf{WSS}) dS \right\|_2 \quad (2.23)$$

and

$$\overline{OSI}_a = \frac{1}{A_a} \int_S (OSI) dS, \quad (2.24)$$

where A_a is the aneurysm surface area.

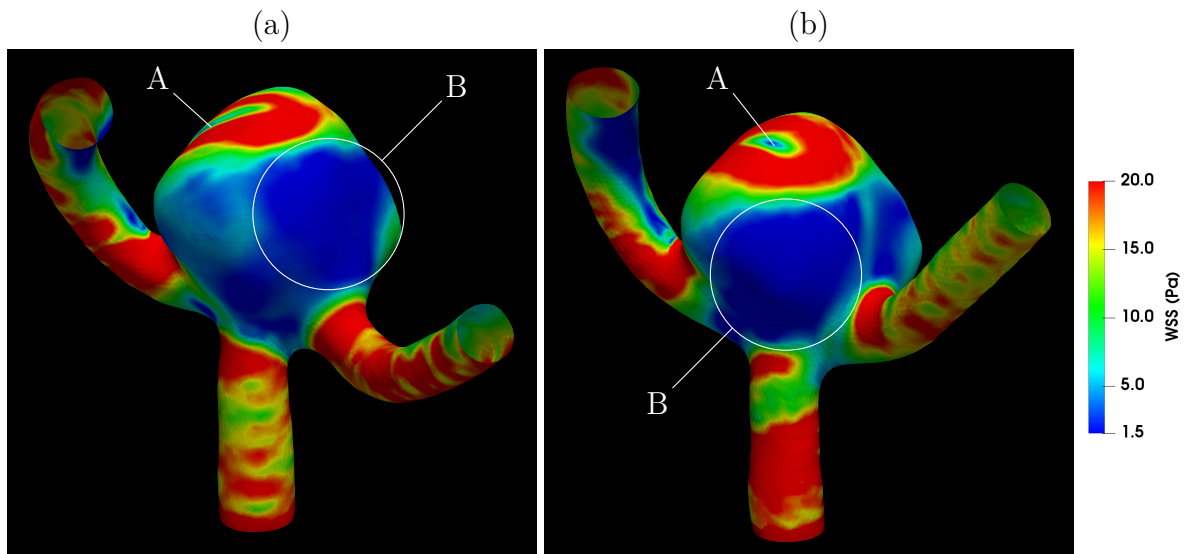
3 RESULTS

In this chapter, we use the results of the numerical simulations to compare the hemodynamics in aneurysms and surrounding arteries for the pre- and post-stent geometries presented in Chapter 2. To ensure numerical accuracy of the simulation data, we performed a mesh and time-step independence study, which is presented in details in Appendix A. Therefore, the following analysis was done using models that were found within an acceptable range of numerical accuracy.

3.1 Case 11

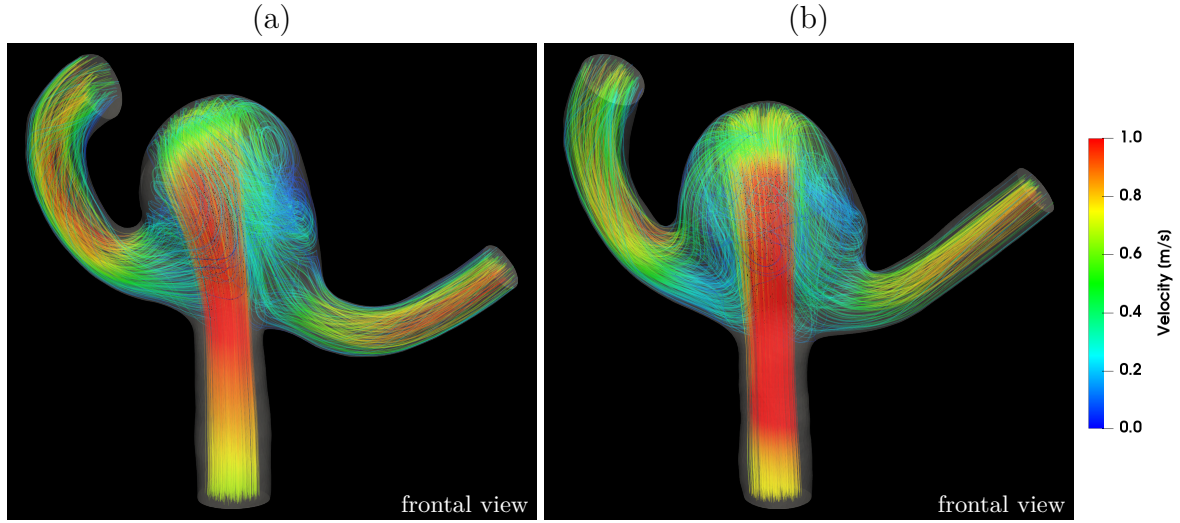
Figures 13 and 14 show the flow pattern and WSS field of the pre- and post-stent geometries of case 11. The lower bound of the WSS scale was set up using a reference value of 1.5 Pa, below which the WSS can degenerate endothelial cells and possibly lead to rupture [23, 25]. Figure 14a shows the flow jet that enters the pre-stent aneurysm sac impinging on the left side of the aneurysm dome, causing a recirculation zone at the opposite side of the aneurysm. The direct impact against the aneurysm wall deflects the flow jet radially, creating a high WSS region—point A in Figure 13a. On the other hand, the low velocity levels of the recirculation flow result in a low WSS area at the right side of the aneurysm sac—point B in Figure 13a.

Figure 13 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case 11 at systolic peak; A and B indicate the flow impingement zone at the dome of the aneurysm and a large area of low WSS ($WSS < 1.5$ Pa), respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surface: 28 Pa and 6.3 versus 29.3 Pa and 7.2, respectively.



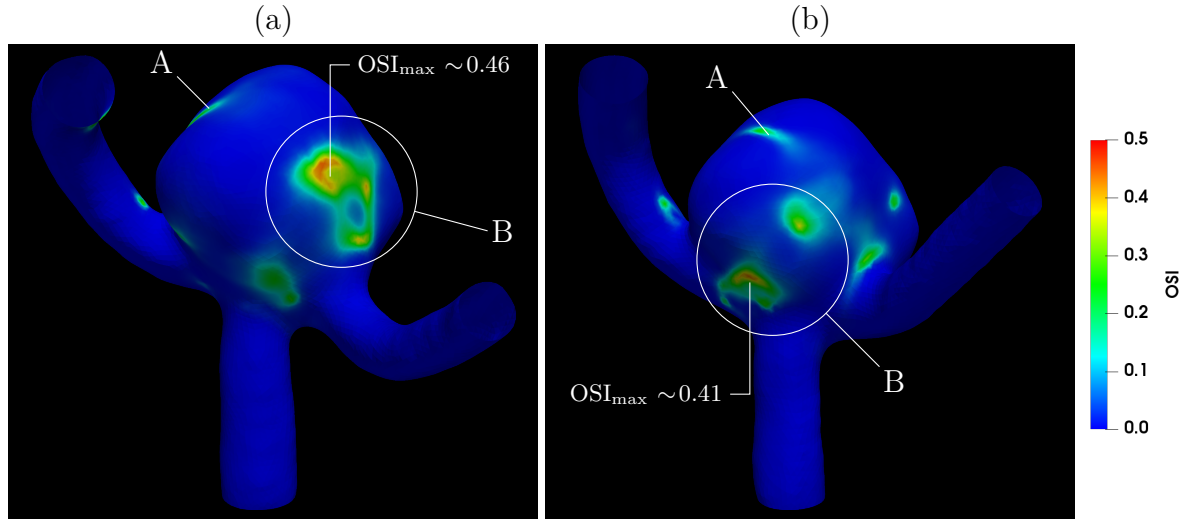
Source: prepared by the author.

Figure 14 – Flow pattern in the (a) pre-stent and (b) post-stent geometries of case 11 at systolic peak.



Source: prepared by the author.

Figure 15 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case 11; A and B indicate high OSI values coinciding with the flow impingement zone at the dome of the aneurysm and a large area of low WSS, respectively. Maximum and mean OSI on the pre- and post-stent aneurysm surfaces: 0.46 and 0.042 versus 0.41 and 0.024, respectively.



Source: prepared by the author.

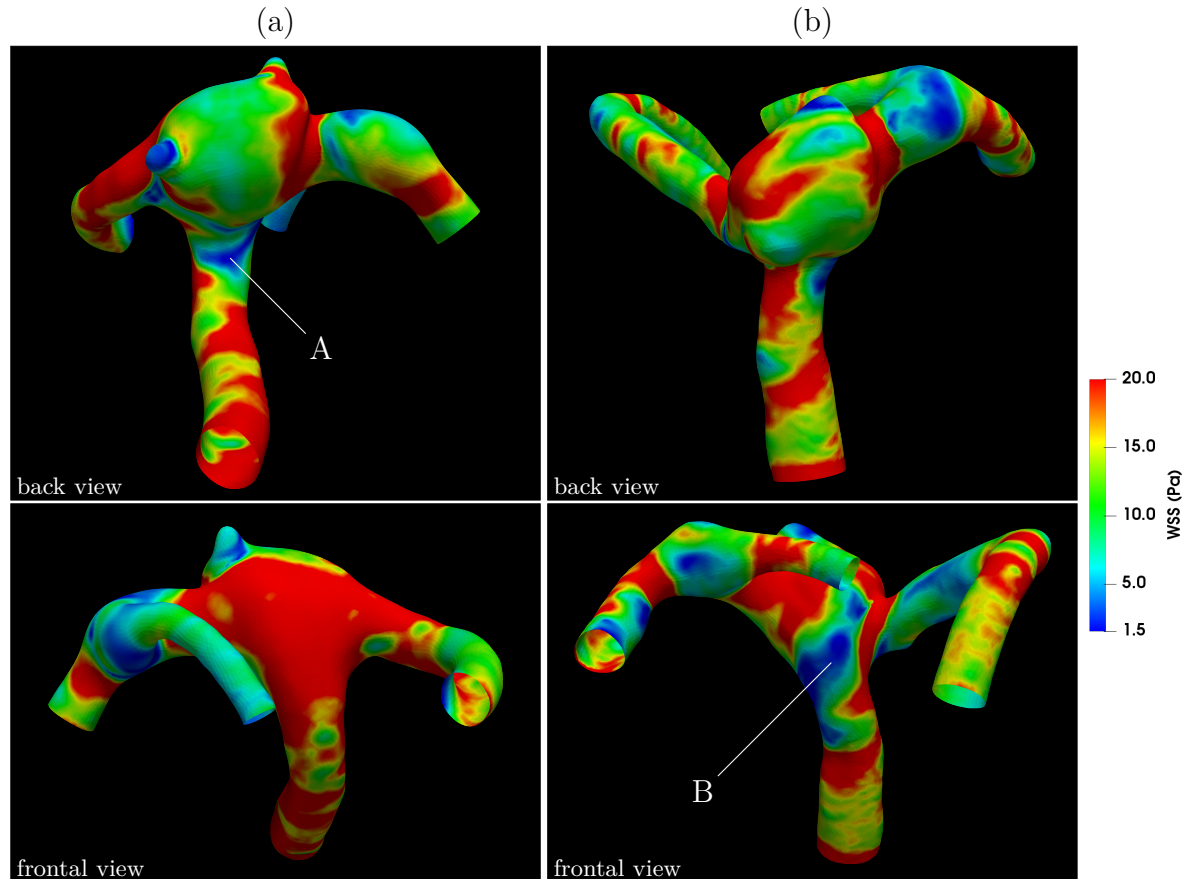
For the post-stent geometry (Figure 14b), we note that the direction of the flow jet entering the aneurysm sac has changed, altering the flow pattern inside the aneurysm. Figure 13 points out a displacement of the low and high WSS regions: both following the changes in flow pattern. Despite the rearrangement of both low and high WSS regions, note that the overall WSS distribution remains similar: the pre-stent aneurysm surface presents a maximum WSS of 28 Pa and a mean WSS of 6.3 Pa; whereas the post-stent aneurysm surface presents a maximum WSS of 29.3 Pa and a mean WSS of 7.2 Pa.

Figure 15 shows the OSI distribution on the pre- and post-stent aneurysms, another important hemodynamic parameter that has been related to aneurysm rupture, specially when combined with low WSS levels [25, 57]. On the pre-stent aneurysm surface, we identify high levels of OSI matching a region of low WSS—point B in Figures 13a and 15a—these could trigger an inflammatory pathway and lead to rupture of the aneurysm. After stent placement, we readily note that the region of high OSI moved away from its early position—point B in Figure 21b. Furthermore, we note a considerable decrease in the OSI levels on the aneurysm surface. This becomes more evident when comparing the mean OSI on the pre- and post-stent aneurysm surfaces: 0.042 and 0.024, respectively.

3.2 Case 16

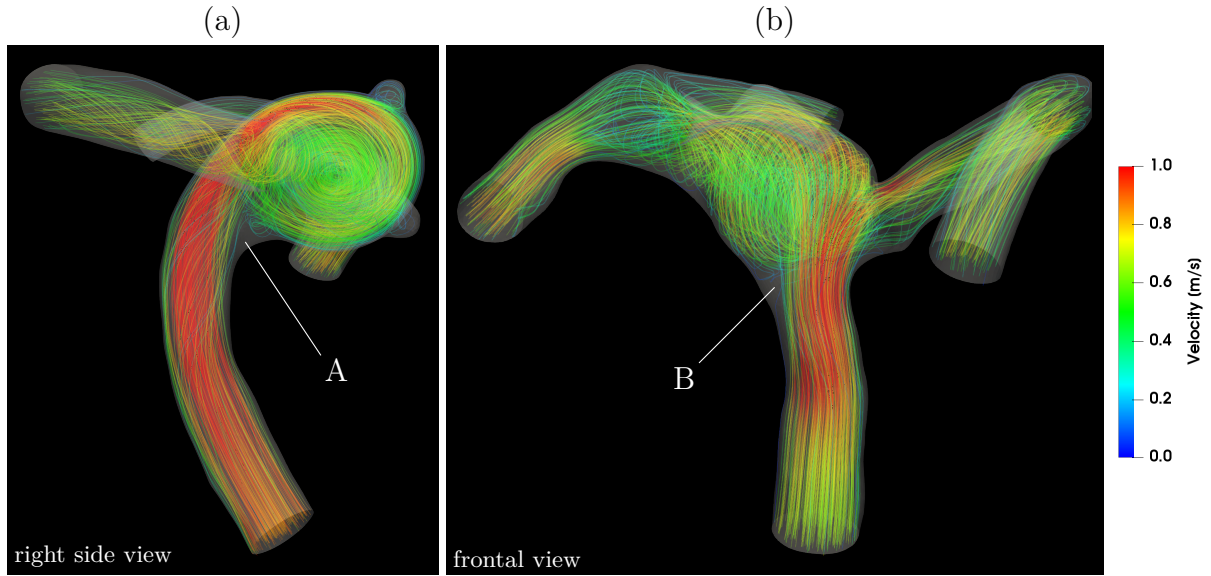
Figures 16 and 17 show the flow pattern and the WSS distribution for the pre- and post-stent geometries of case 16. In Figure 16 we identify a large area of high WSS covering the frontal wall of the parent artery, the aneurysm dome, and daughter arteries. Analyzing

Figure 16 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case 16 at systolic peak; A and B indicate a low WSS region on the pre- and post-stent surfaces, respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surfaces: 47.3 Pa and 15 Pa versus 57.7 Pa and 17.1 Pa, respectively.



Source: prepared by the author.

Figure 17 – Flow pattern in aneurysm case 16 at systolic peak: (a) side view of the pre-stent geometry and (b) frontal view of the post-stent geometry. Points A and B indicate a slow recirculation flow causing a low WSS region on both surfaces.



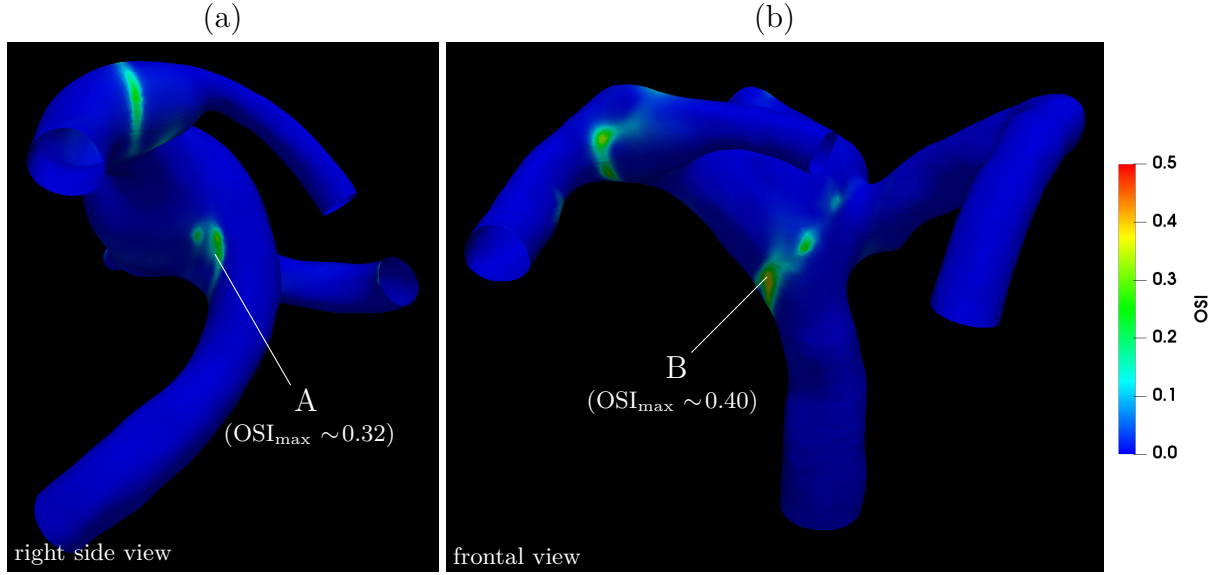
Source: prepared by the author.

the flow pattern in the pre-stent geometry (Figure 17a) reveals the flow “washing” the frontal wall of the aneurysm, which leads to high velocity gradients adjacent to the wall. Furthermore, we identify a separating flow due to the curved geometry of the parent artery, which causes a recirculation flow zone, resulting in a low WSS area—point A in Figures 16a and 17a.

For the post-stent geometry, Figure 16b shows a similar WSS distribution on the aneurysm surface. However, we identify two main differences. First, the low WSS region moved from the back to the left side of the parent artery, indicated by point B in Figure 16b. An analysis of the flow pattern in the post-stent geometry (Figure 17b) shows that the separating flow was dislocated due to straightening of the parent artery. Second, we note a smaller area of high WSS on the aneurysm surface, resulting in a smaller mean WSS on the aneurysm: 17.1 Pa for the pre-stent geometry versus 15 Pa for the post-stent geometry. Despite the reduction in the mean WSS, higher WSS levels are found on the post-stent surface rather than on the pre-stent surface: 57.7 Pa versus 47.3 Pa.

Regarding the OSI field, Figure 18 shows the values for both geometries. We easily identify an area of high OSI matching the region of low WSS on both pre- and post-stent geometries, which might increase the risk of rupture [25]. Moreover, in Figure 18 we identify an increase in the maximum OSI values found on the pre- (0.32) versus post-stent (0.40) surfaces. Nonetheless, the mean OSI remains almost unaltered (0.007 versus 0.008).

Figure 18 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case 16. Point A indicates elevate OSI levels coinciding with a low WSS region ($WSS < 1.5$ Pa). Maximum and mean OSI on the pre- and post-stent aneurysm surfaces: 0.32 and 0.007 vs 0.40 and 0.008, respectively.

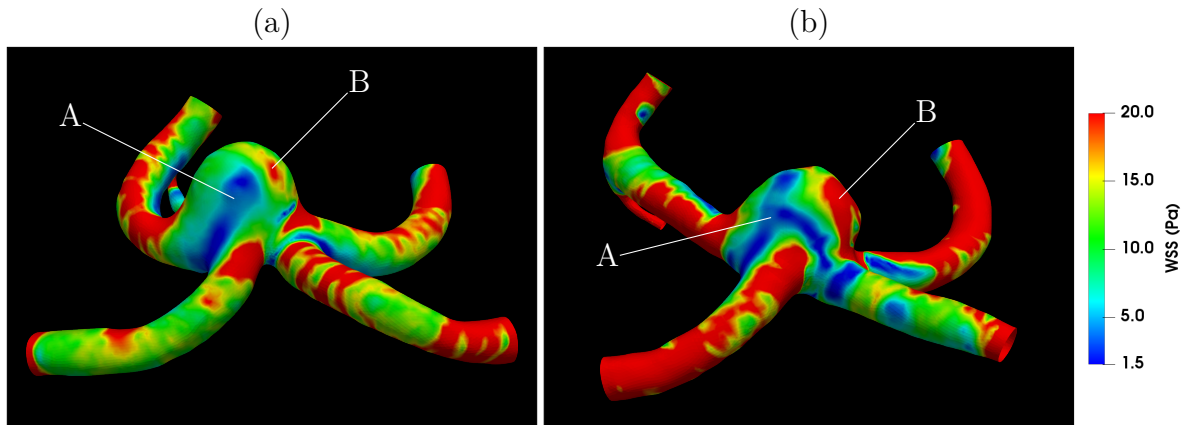


Source: prepared by the author.

3.3 Case 17

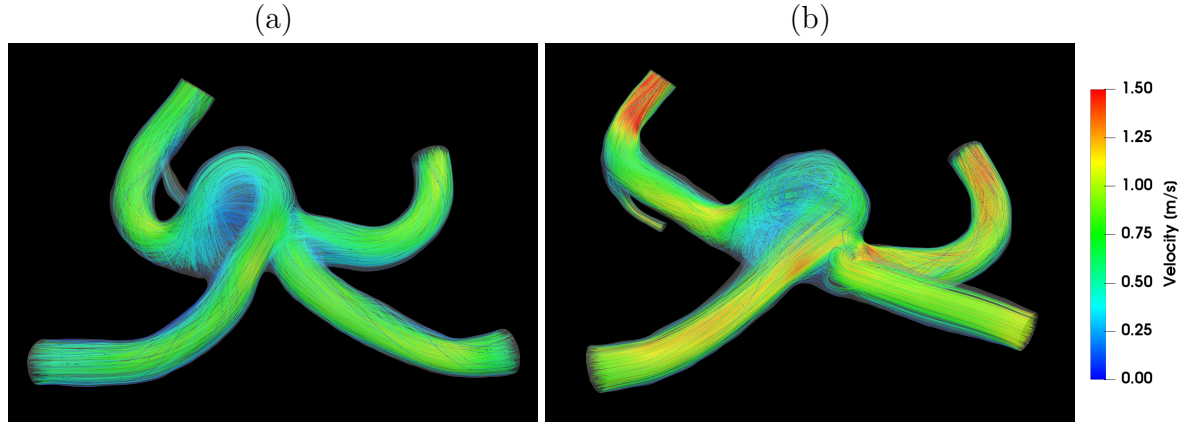
The WSS field and the flow pattern for the pre- and post-stent geometries of case 17 are presented in Figures 19 and 20, respectively. Comparing the WSS field on the pre- and post-stent surfaces, we note an increase in WSS levels on the aneurysm surface and specially on the surrounding arteries. Such change can be explained analyzing the flow

Figure 19 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case 17 at systolic peak; A and B indicate areas of low and high WSS on the aneurysm sac, respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surfaces: 49.4 Pa and 11.5 Pa versus 81.2 Pa and 18.5 Pa, respectively.



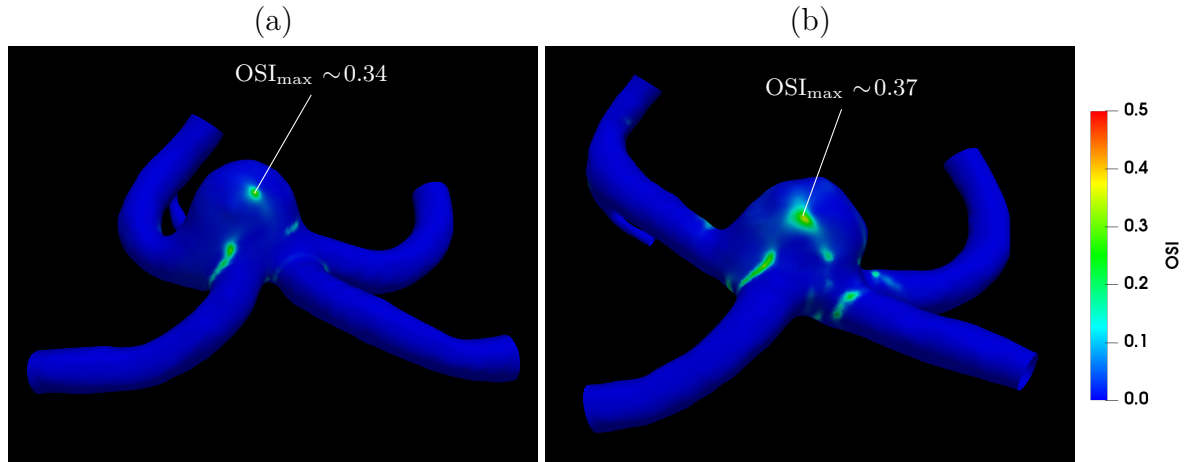
Source: prepared by the author.

Figure 20 – Flow pattern in the (a) pre-stent and (b) post-stent geometries of case 17 at systolic peak.



Source: prepared by the author.

Figure 21 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case 17. Maximum and mean OSI on the pre- and post-stent aneurysm surfaces: 0.34 and 0.012 versus 0.37 and 0.015, respectively.



Source: prepared by the author.

pattern, shown in Figure 20. In the pre-stent geometry, the left parent artery contributes almost exclusively to the blood flow into the aneurysm. The flow “washes” the aneurysm surface and flows into the left daughter artery. This causes a recirculation flow to appear, resulting in a low WSS region. In addition, due to the angular configuration of the arteries, the flow from the right parent artery is smoothly deflected to the right daughter artery. For the post-stent geometry, we note a similar behavior; however, due to the angular remodeling, the new configuration causes the flow from the right parent artery to be deflected in a more abrupt manner, resulting in greater flow activity in the aneurysm and higher levels of WSS—point B in Figure 19a.

In sum, the mean WSS increased from 11.5 Pa to 18.5 Pa after stenting. Such increase is not only related to an increase in the area of high WSS but also to higher

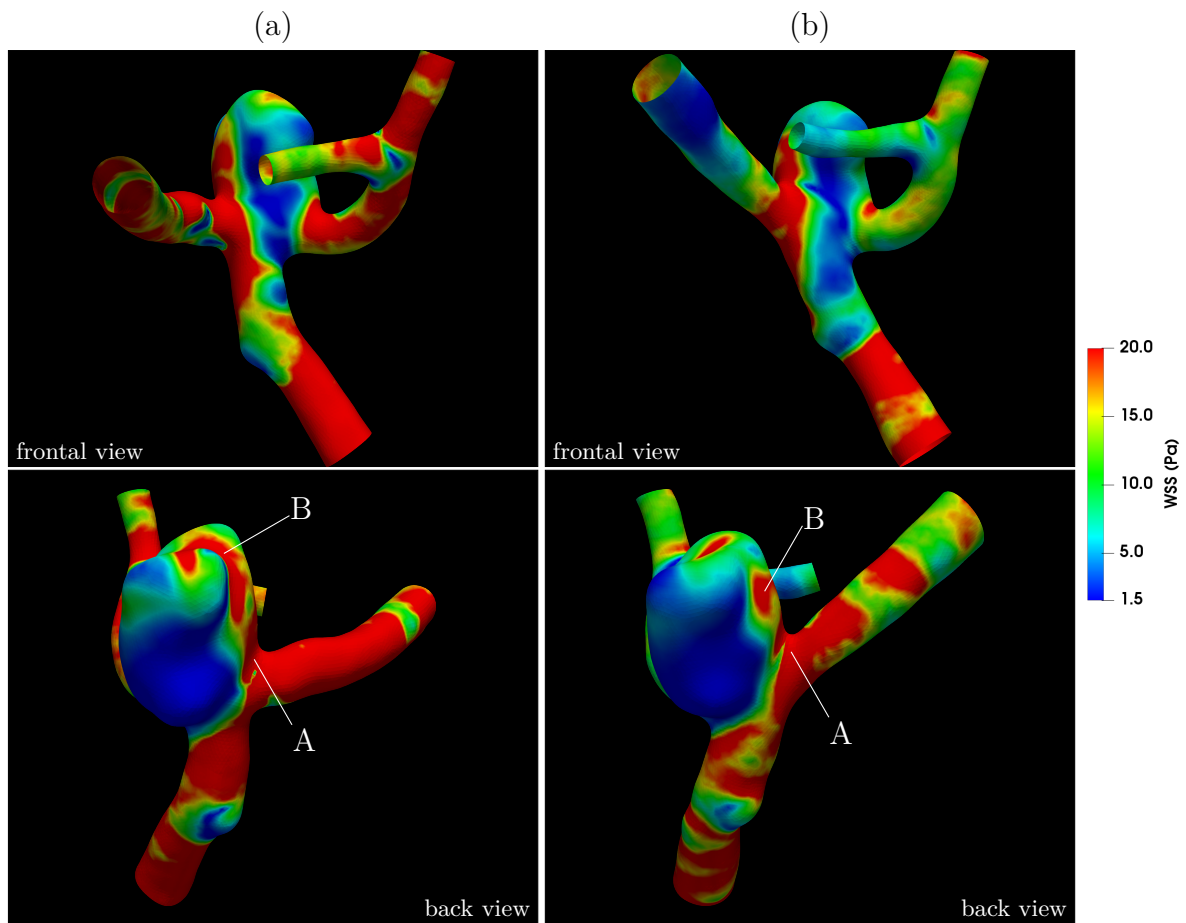
WSS levels, which increased by approximately 65%: going from a maximum of 49.4 Pa to 81.2 Pa on the high WSS region indicated by point B in Figure 19.

Figure 21 shows a comparison of the OSI field on the pre- and post-stent surfaces of case 17. Like the changes in the WSS field, the OSI level increased after stent placement. The maximum OSI on the aneurysm increased after stenting, going from 0.34 to 0.37. The same occurred for the mean OSI, which increase from 0.012 to 0.015.

3.4 Case E1

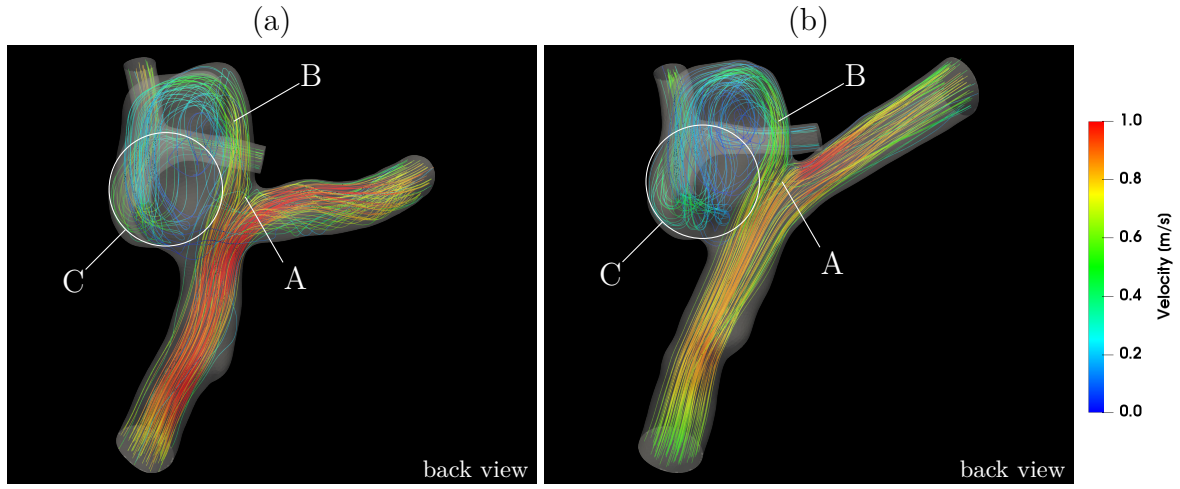
Figures 22 and 23 show the WSS field and flow pattern for the pre- and post-stent geometries of case E1. Analyzing the WSS distribution on the pre-stent geometry, we note a region of high WSS on the side of the aneurysm indicated by points A and B. From the flow pattern (Figure 23) we identify this region as the FIZ, on which the flow from the

Figure 22 – WSS field on the (a) pre-stent and (b) post-stent surfaces of case E1 at systolic peak. Point A and B indicate a region of high WSS due to flow impingement against the aneurysm neck and a region of high WSS on the aneurysm dome, respectively. Maximum and mean WSS on the pre- and post-stent aneurysm surfaces: 77.3 Pa and 10.8 Pa versus 47.4 Pa and 9.4 Pa, respectively.



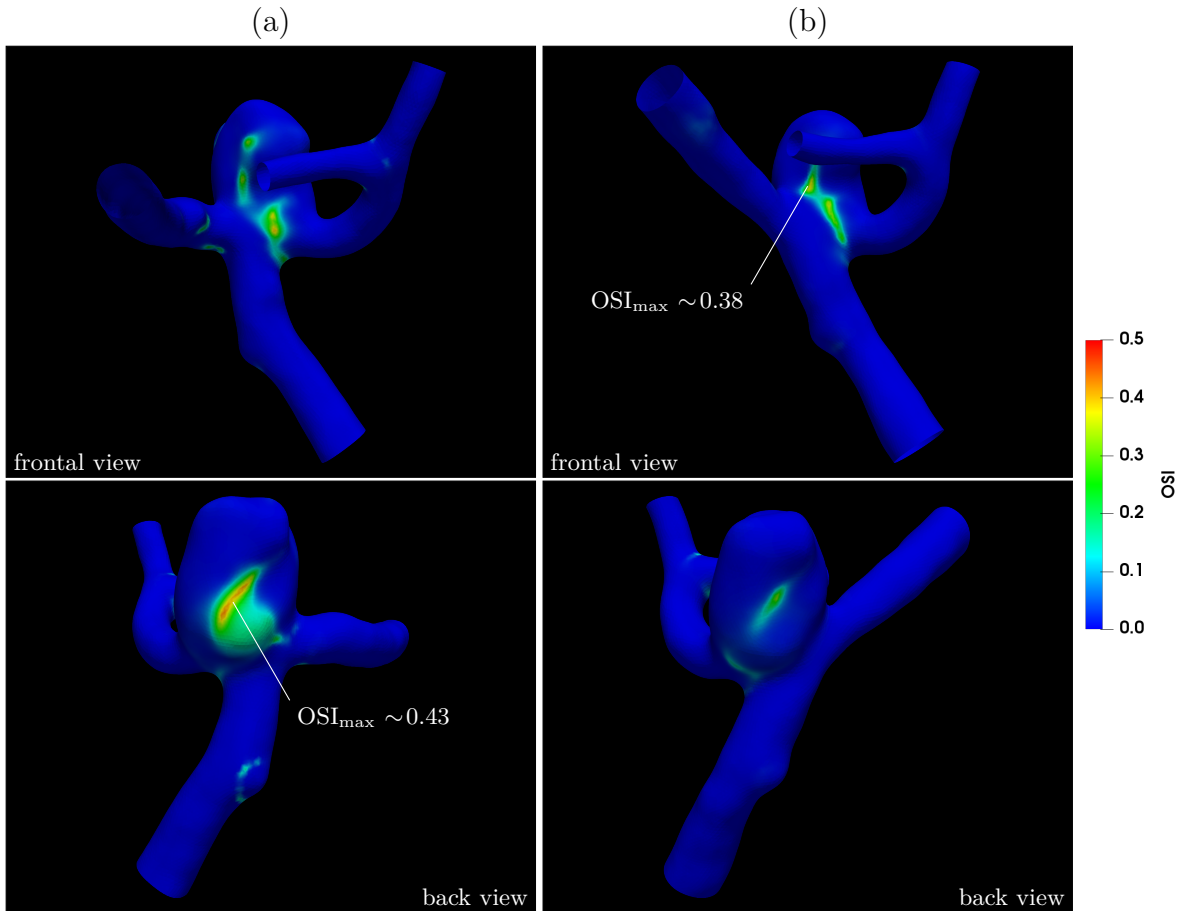
Source: prepared by the author.

Figure 23 – Flow pattern in the (a) pre-stent and (b) post-stent geometries of case E1 at systolic peak. Point A and B indicate a splitting flow region and the flow jet entering the aneurysm; Point C indicates a large recirculation flow zone at the aneurysm fundus.



Source: prepared by the author.

Figure 24 – OSI field on the (a) pre-stent and (b) post-stent surfaces of case E1. Maximum and mean OSI on the pre- and post-stent aneurysm surfaces: 0.43 and 0.026 versus 0.38 and 0.013, respectively.



Source: prepared by the author.

parent artery impinges and splits into two streams: one flowing into the aneurysm and other into the daughter artery. Furthermore, point C indicates a recirculation flow zone at the aneurysm fundus, resulting in a large region of low WSS on the back of the aneurysm.

After stent placement, the vascular remodeling straightened the arteries, increasing the blood flow rate into the daughter artery, therefore, decreasing the blood flow rate into the aneurysm, as seen in Figure 23b. Because of lower flow activity in the aneurysm, we note a reduction in the WSS levels on the aneurysm sac, which becomes more evident when comparing the maximum and mean WSS levels on the pre- and post-stent aneurysm surfaces: 77.3 Pa and 10.8 Pa versus 47.4 Pa and 9.4 Pa, respectively.

Regarding the OSI field on the pre- and post-stent geometries (Figure 24), we readily note a reduction in the OSI levels, specially on the aneurysm back. After stenting, the maximum OSI on the aneurysm went from 0.43 to 0.38 and the mean OSI decreased by 50% (0.026 versus 0.013). Note also that while a lower flow activity in the aneurysm sac increased the extent of the low WSS region on the back of the aneurysm, it also decreased the OSI levels on the very same region, which in turn decreases the risk of rupture [25].

Finally, Table 3 shows a summary of maximum and mean values of both WSS and OSI on the pre- and post-stent aneurysm surface of each case presented above.

Table 3 – Comparison of maximum and mean values of WSS and OSI on the pre- and post-stent aneurysm surfaces of case 11, case 16, case 17, and case E1.

Case		WSS (Pa)		OSI (-)	
		Maximum	Mean	Maximum	Mean
Case 11	pre-stent	28	6.3	0.46	0.042
	post-stent	29.3	7.2	0.41	0.024
Case 16	pre-stent	47.3	17.1	0.32	0.007
	post-stent	57.7	15.0	0.40	0.008
Case 17	pre-stent	49.4	11.5	0.34	0.012
	post-stent	81.2	18.5	0.37	0.015
Case E1	pre-stent	77.3	10.8	0.43	0.026
	post-stent	47.4	9.4	0.38	0.013

Source: prepared by the author.

4 DISCUSSION AND CONCLUSIONS

Throughout the last decade, stent-assisted coil embolization of intracranial aneurysms have achieved widespread acceptance, with different variants being constantly proposed. In the two-step Y-stent coiling of bifurcation aneurysms, stenting and coiling are done in separate steps; in between these steps, stent-induced vascular remodeling has been speculated to play an important role, altering the hemodynamics in the aneurysm sac. However, it is still unknown whether this two-step approach could benefit from the vascular remodeling caused by the placement of stents.

The current work sought to elucidate the role of stent-induced vascular remodeling in modifying the hemodynamics of bifurcation aneurysms. Table 4 shows a summary of our findings. Our results support previous suspicions reported in the literature, showing that in fact stent-induced vascular remodeling alters the hemodynamics in the aneurysm sac; moreover, vascular remodeling showed a variable effect in modifying the hemodynamics. The number of cases presented in the current study is not sufficient to draw definitive conclusions regarding the effects of stent-induced vascular remodeling on the hemodynamics of bifurcation aneurysms; therefore, interpretation of these findings requires caution. Nonetheless, an analysis of these cases may provide a better understanding of the consequences of hemodynamic changes in the aneurysm sac.

Table 4 – Summary of the findings of the current work. WSS and OSI values expressing the percent variation after vascular remodeling.

Aneurysm location	Parent artery	Stent configuration	Maximum WSS (%)	Mean WSS (%)	Maximum OSI (%)	Mean OSI (%)
ACoA bifurcation	left and right ACA	single stent	80.8	60.2	8.8	25
MCA bifurcation	MCA	Y-stent	4.6	14.2	-10.9	-42.9
MCA bifurcation	MCA	Y-stent	21.9	-12.3	25	14.3
MCA bifurcation	MCA	single stent	-38.7	-12.9	-11.6	-50

Source: prepared by the author.

Since the first clinical reports on stent-induced vascular remodeling, authors have speculated that vessel straightening could promote a favorable hemodynamic environment in the aneurysm sac, contributing to the aneurysm healing process. However, in the present study one of the cases—at the ACoA bifurcation—showed an adverse hemodynamic response to the novel vascular geometry, contradicting those suspicions. ACoA bifurcation aneurysms are under the influence of two parent arteries: left and right branches of the ACA, both arriving at the ACoA bifurcation parallel to each other. By straightening the vessels, the novel vascular geometry may cause the parent arteries to lay in a perpendicular-like configuration. In our study, this was observed to induce a greater flow instability in

the aneurysm sac, increasing hemodynamic parameters associated with aneurysm rupture. Nonetheless, further investigation is necessary to determine whether this is a common behavior for aneurysms at the ACoA bifurcation.

Recent studies have shown that a hands-up vascular configuration in bifurcation aneurysms—i.e., a Y-like vascular geometry—leads to rupture more often than other vascular geometries. In our study, two aneurysms at bifurcations of the MCA were treated with Y-stent technique, resulting in a Y-like vascular geometry. A Y-like geometry aligns the parent artery and aneurysm ostium; thus, producing a straight flow jet that impinges directly on the aneurysm dome. In both cases, this was observed to increase the maximum WSS levels at the flow impingement zone. An increase in WSS levels may accelerate its destructive effect on the aneurysm surface, increasing the risk of rupture.

Both aneurysms treated with Y-stenting showed an adverse hemodynamic response to the novel Y-like vascular geometry. However, our results do not consider the presence of coils. In the literature, clinical reports have shown that Y-stent coiling is effective in healing the aneurysm, reducing rates of recanalization and recurrence. Moreover, numerical studies have shown that the effectiveness of Y-stent coiling is associated with a combined effect of vascular remodeling and the presence of a coil mass inside the aneurysm sac: the Y-like vascular geometry redirects the flow jet towards the aneurysm ostium, where the coil mass is located—an inert, nonbiologically active surface that is not affected by the destructive effect of high WSS levels. Therefore, considering these scenarios, it would not be recommended to perform Y-stenting and coiling in separate steps.

One of the aneurysms at the MCA bifurcation was initially treated with a single stent. In bifurcation aneurysms, placement of single stent leads to straightening of the parent-daughter artery segment hosting the stent, which approximates the novel vascular geometry to the one of a sidewall aneurysm. In sidewall aneurysms, stent-induced vascular remodeling has been shown to reduce the blood flow rate into the aneurysm, which reduces flow activity in the aneurysm sac. In this case, we observed a similar effect. Straightening of the daughter artery led to a reduction in the blood flow rate into the aneurysm, which reduced the flow activity in the aneurysm sac. Moreover, due to lower flow activity in the aneurysm sac, WSS and OSI levels decreased by up to 50%, which may delay the destructive effect of the WSS and OSI on the aneurysm surface.

One of the limitation of the present study is related to the absence of stent struts covering the aneurysm ostium. Stent struts act as momentum sinks, reducing flow velocity inside the aneurysm sac; therefore, modifying the intraaneurysmal hemodynamics. Another limitation of the present study is related to the assumption of rigid vessel walls, which have been proven to influence the intraaneurysmal hemodynamics. However, due to the presence of a continuous outward-directed radial force, stents may increase stress in the vessel wall and interfere in wall functions—specially wall movement. Therefore, further investigation is necessary to elucidate the influence of stents on vessel wall movement.

Future works should explore the presence of stent struts covering the aneurysm ostium in order to achieve a better understanding of the combined influence of stent-induced vascular remodeling and stent struts on intraaneurysmal hemodynamics. In addition, the assumptions of fixed outlet pressure and blood as Newtonian fluid should be re-evaluated. Different assumptions—such as non-Newtonian fluid models and time-varying pressure conditions—have been proposed in the literature and should be explored.

Despite the limitations of the present study, we were able to elucidate aspects related to stent-induced vascular remodeling that were previously unknown. In conclusion, hemodynamics change in intracranial aneurysms due to stent-induced vascular remodeling. Therefore, stent-assisted treatments may benefit—or not—from the novel vascular remodeling. In two-step Y-stent coiling, placement of a single stent in an earlier step reduces hemodynamic parameters related to aneurysm rupture during the “healing-in” process of the stent. Another important conclusion of the current work regards the variable effect of stent-induced vascular remodeling in modifying the hemodynamics. Contrary to previous suspicions, straightening of the host vessels may also induce an adverse hemodynamic environment. This was observed to occur in aneurysms at the ACoA bifurcation.

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Appendices

A – MESH AND TIME-STEP INDEPENDENCE STUDY

In a numerical simulation, we must assess the accuracy and reliability of the simulation results. To this end, validation and verification (V&V) present a number of recommendations and guidelines [58]. In V&V, validation refers to physical test of the mathematical model adopted to describe the problem. Unfortunately, we were unable to validate the results due to lack of experimental data on aneurysms; we leave the task of setting up an physical test for blood flow in aneurysms as a suggestion for future works.

On the other hand, verification aims to assess the accuracy and correctness of the mathematical model implementation, i.e., temporal and spatial resolution, discretization method of the governing equations, and code implementation. Regarding code implementation, OpenFOAM uses the FVM, a well established and consolidated method for discretizing partial differential equations in the form of algebraic equations. Furthermore, OpenFOAM has an active community of developers and is widely used in both academic and industrial research, being constantly audited, tested, and benchmarked. For these reasons, we consider the code verified.

To assess numerical accuracy of temporal and spatial resolution, we carried out a mesh and time-step independence study considering two parameters: the spatial distribution of WSS on the surface at systolic peak, which represents the instant of maximum blood flow rate in the parent artery; and the area-averaged WSS over the wall surface, defined as

$$\overline{WSS}_S = \frac{1}{A_S} \left\| \int_S \mathbf{WSS} dS \right\|_2, \quad (\text{A.1})$$

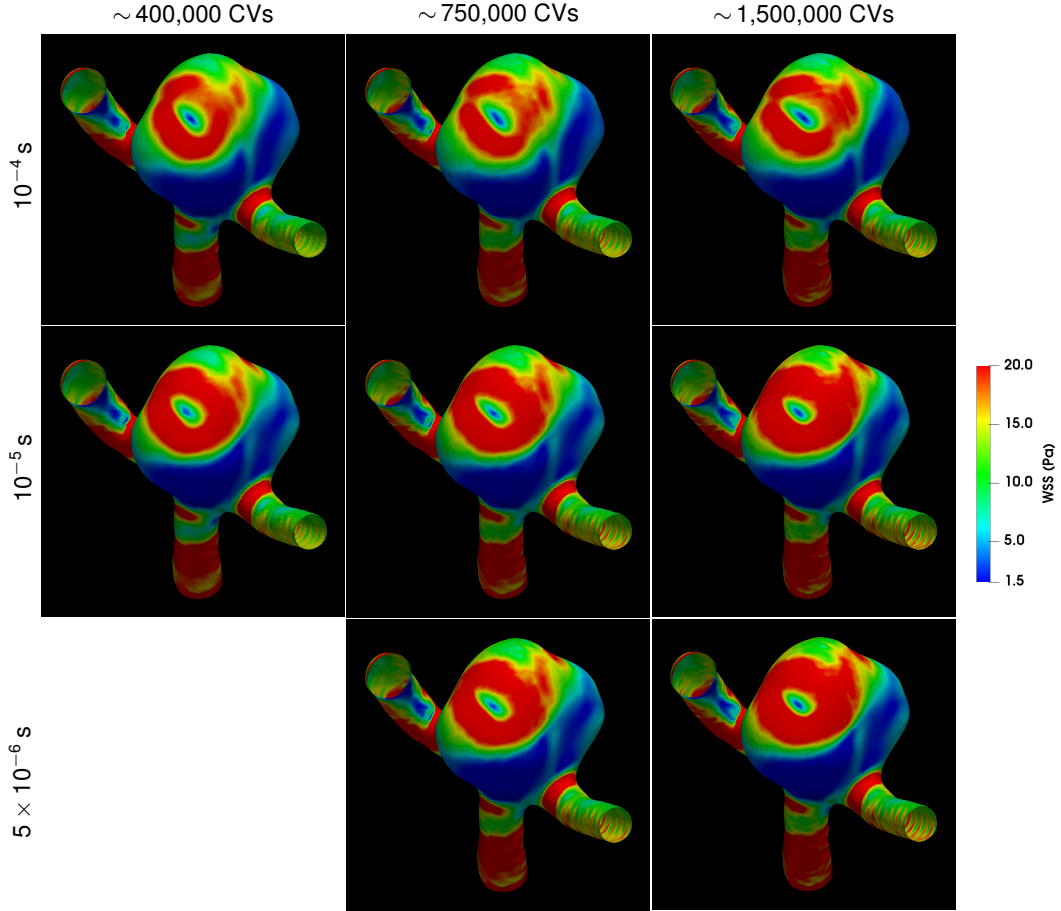
where S is the wall surface and A_S its area. Further, because of the unique flow pattern due to geometric features of the aneurysm [45], we share the idea that each patient-specific geometry requires its own mesh and time-step independence study [59]. Therefore, we performed a separate analysis for each one of the cases in our research, as presented in the following sections.

A.1 Case 11

Post-stent

Figure 25 shows the WSS field on the post-stent surface of case 11 for meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s. Observing the time-steps 10^{-4} s and 10^{-5} s, we note qualitative differences in the WSS field; on the other hand, we see the same WSS field when comparing time-steps

Figure 25 – Mesh and time-step independence analysis for the post-stent geometry of case 11: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.



Source: prepared by the author.

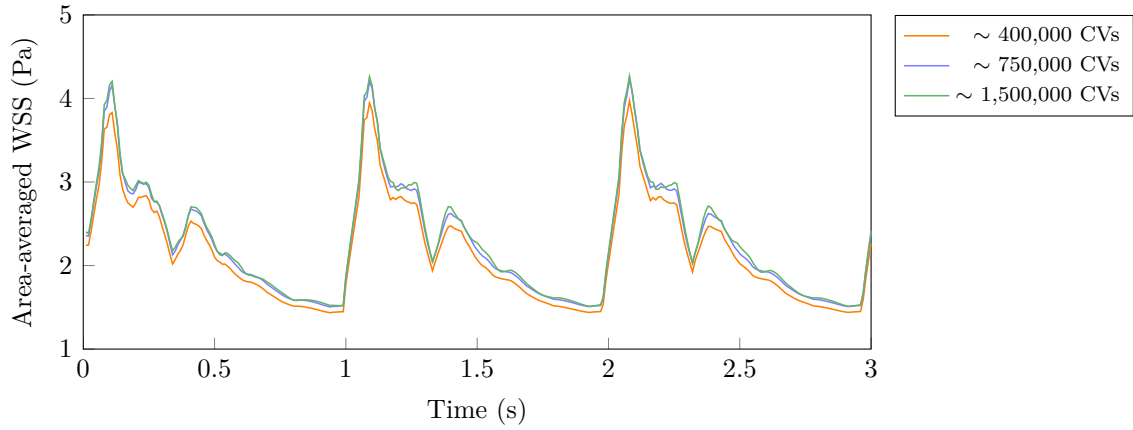
10^{-5} s and 5×10^{-6} s, suggesting that a time-step of 10^{-5} is adequate to represent the blood flow in this geometry.

Regarding spatial resolution, Figure 25 shows a similar WSS field when comparing the meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ for a time-step of 10^{-5} s. However, analyzing the area-averaged WSS for these meshes (Figure 26), we note the same profile for both higher-order meshes, indicating that $\sim 750,000$ control volumes along with a time-step of 10^{-5} s are adequate to establish the overall blood flow pattern in this geometry.

Pre-stent

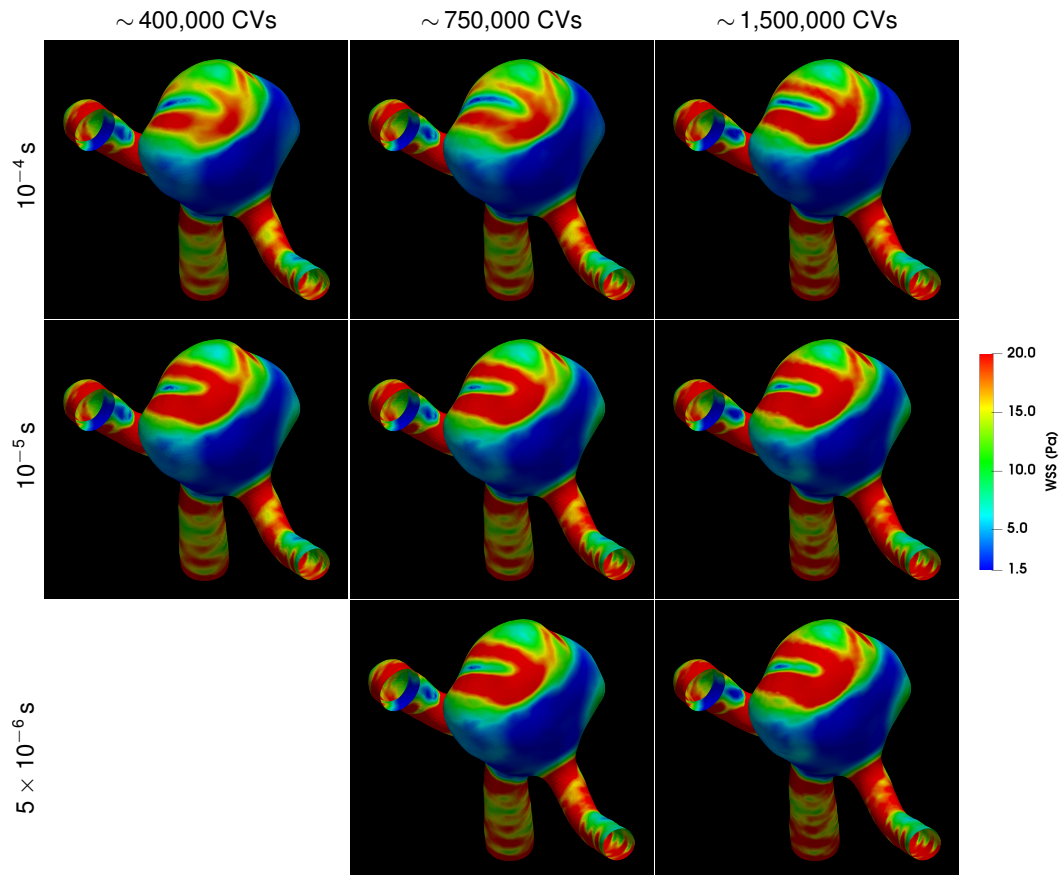
Following the same procedure, we first evaluated the WSS field on the pre-stent surface of case 11 (Figure 27) and established 10^{-5} s as an adequate temporal resolution. As for the spatial resolution, a qualitative analysis of the WSS field shows no considerable differences. The same occurs when comparing the area-averaged WSS (Figure 28). At peak systole, the difference is about 10% between the meshes $\sim 400,000$ and $\sim 1,500,000$ and only 4%

Figure 26 – Area-averaged WSS on the post-stent surface of case 11 as a function of time for meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.



Source: prepared by the author.

Figure 27 – Mesh and time-step independence analysis for the pre-stent geometry of case 11: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.

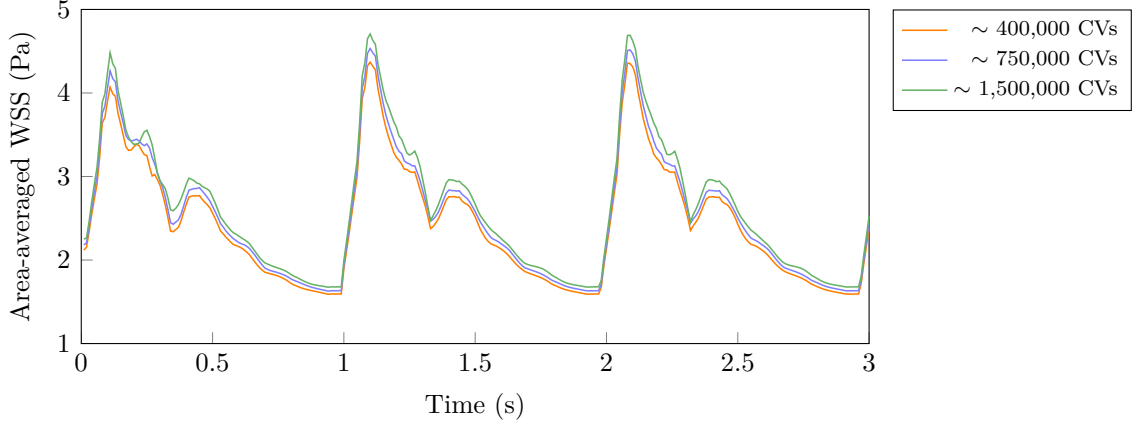


Source: prepared by the author.

between the two higher-order meshes.

Although the lower-order mesh can represent the flow and WSS fields within a reasonable range of tolerance, we adopted the mesh with $\sim 750,000$ control volumes in our analysis in order to maintain consistency with the post-stent mesh resolution.

Figure 28 – Area-averaged WSS on the pre-stent surface of case 11 as a function of time for meshes with $\sim 400,000$, $\sim 750,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.



Source: prepared by the author.

A.2 Case 16

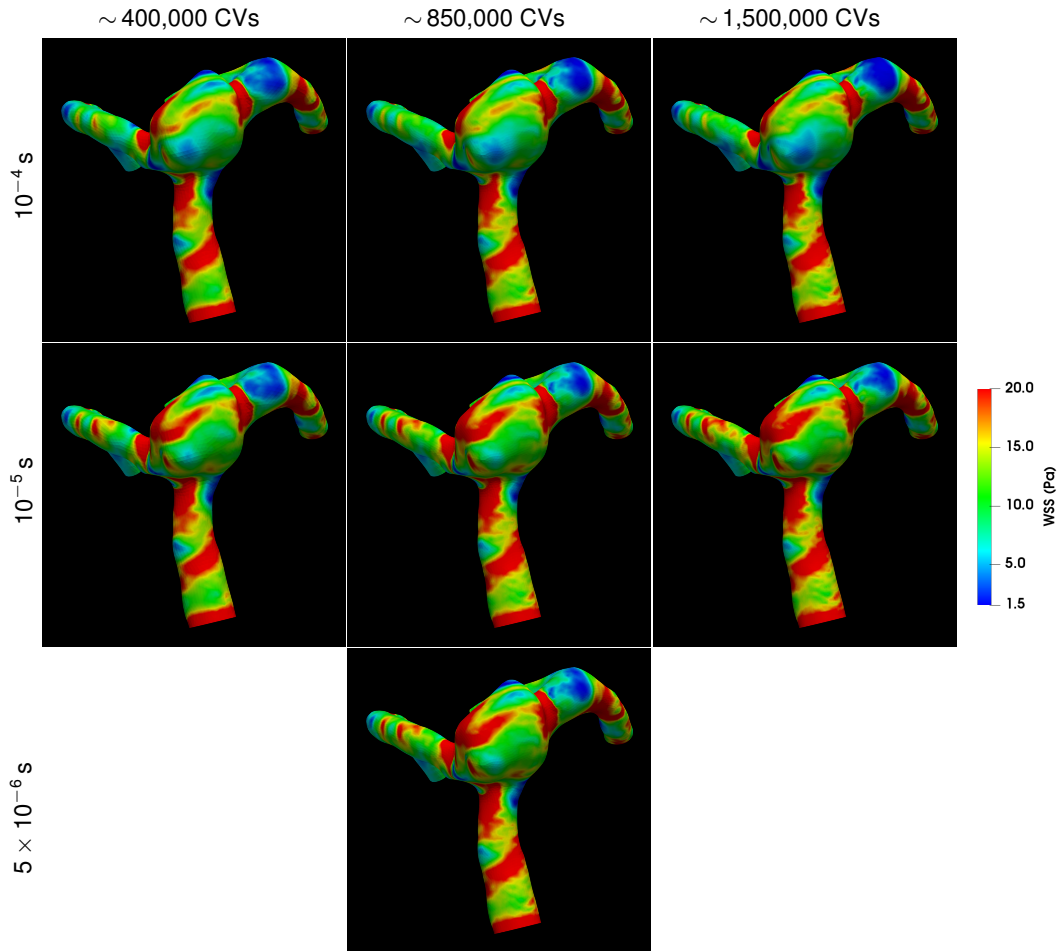
Post-stent

For the post-stent geometry of case 16, the WSS field remains unaltered when comparing pairwise $\sim 850,000$ control volumes, 10^{-5} s to higher temporal and spatial resolutions, as seen in Figure 29. Similar results are observed even with a mesh size of $\sim 400,000$ control volumes. However, a comparison of the area-averaged WSS profiles (Figure 30) shows $\sim 850,000$ control volumes in much closer agreement with a higher-order refinement level than $\sim 400,000$ control volumes; thereby, we adopted a spatial and temporal discretization of $\sim 850,000$ control volumes and 10^{-5} s, respectively.

Pre-stent

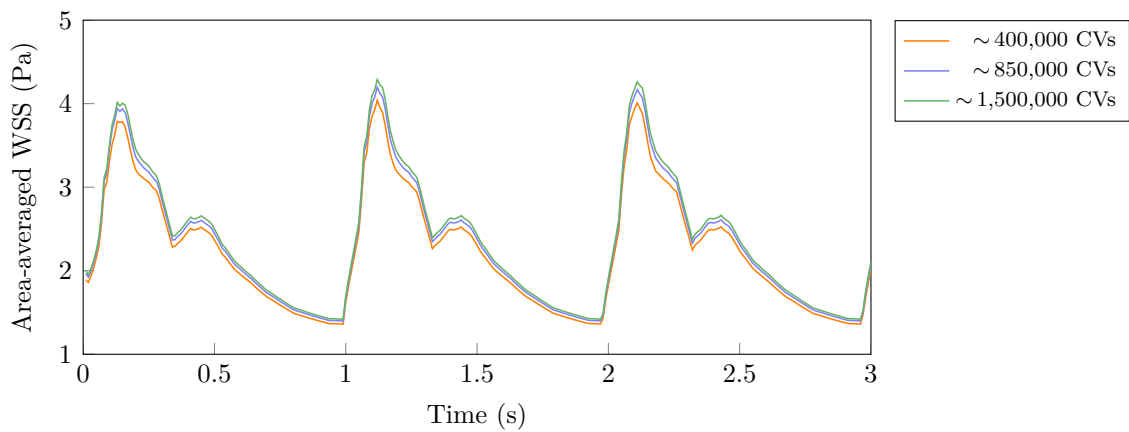
As for the pre-stent geometry of case 16, we note similar WSS fields comparing meshes with $\sim 850,000$ and $\sim 1,500,000$ control volumes for time-steps of 10^{-5} s and 5×10^{-6} s (Figure 31), indicating convergence of temporal discretization. Regarding spatial resolution, we note in Figure 32 the profiles in close agreement but not entirely coincident when comparing the three meshes for a time-step of 10^{-5} s; even though, the difference between the two highest refinement levels at systolic peak is about 4%, which we consider negligible.

Figure 29 – Mesh and time-step independence analysis for the post-stent geometry of case 16: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.



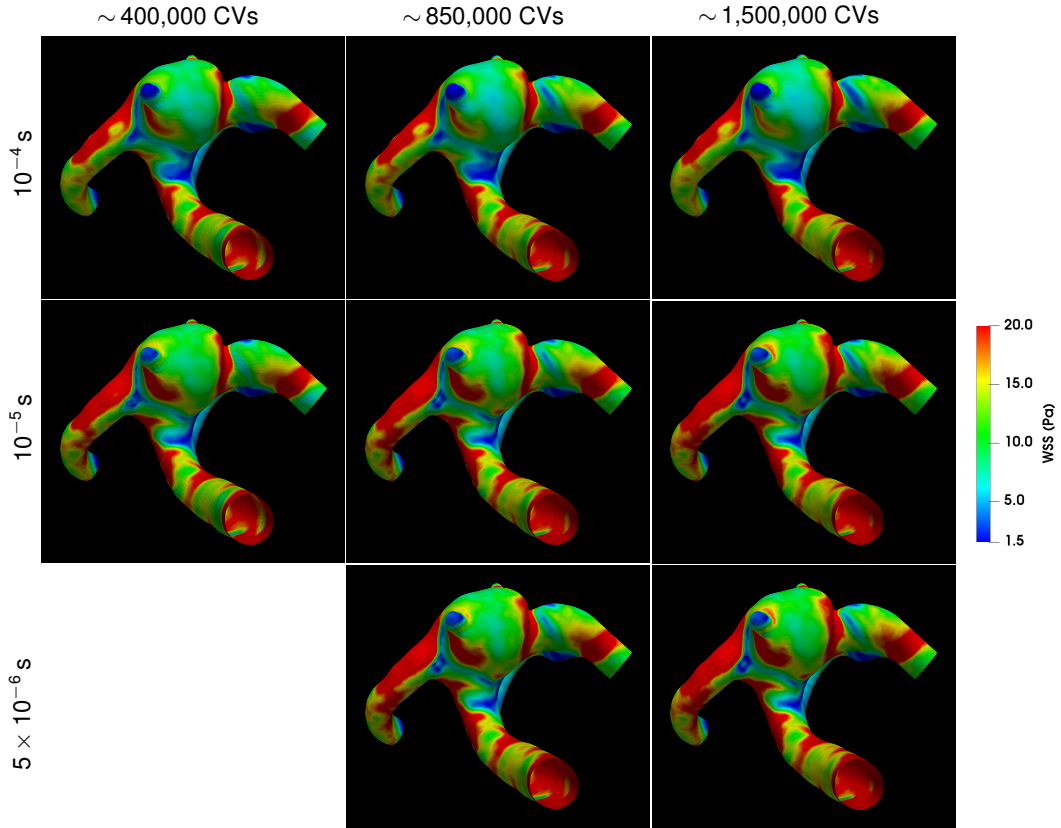
Source: prepared by the author.

Figure 30 – Area-averaged WSS on the post-stent surface of case 16 as a function of time for meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.



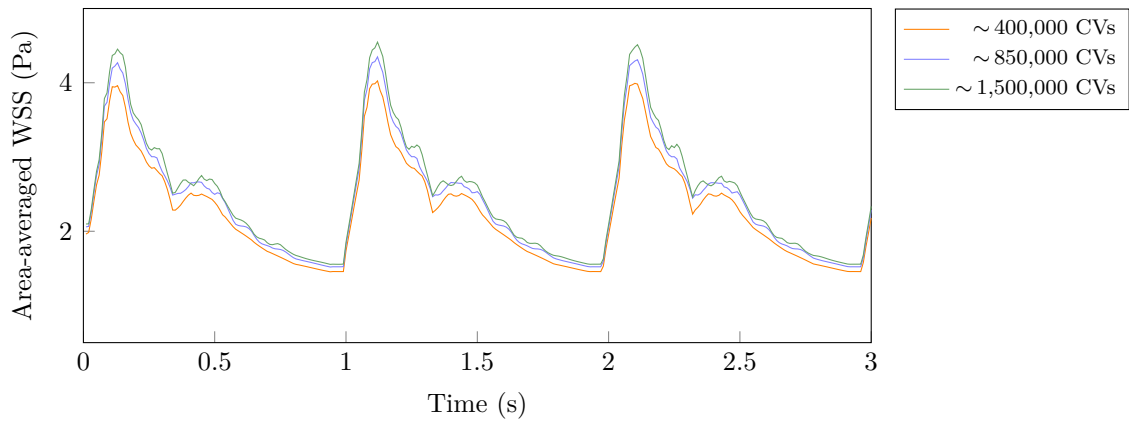
Source: prepared by the author.

Figure 31 – Mesh and time-step independence analysis for the pre-stent geometry of case 16: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.



Source: prepared by the author.

Figure 32 – Area-averaged WSS on the pre-stent surface of case 16 as a function of time for meshes with $\sim 400,000$, $\sim 850,000$, and $\sim 1,500,000$ control volumes and time-step of 10^{-5} s.



Source: prepared by the author.

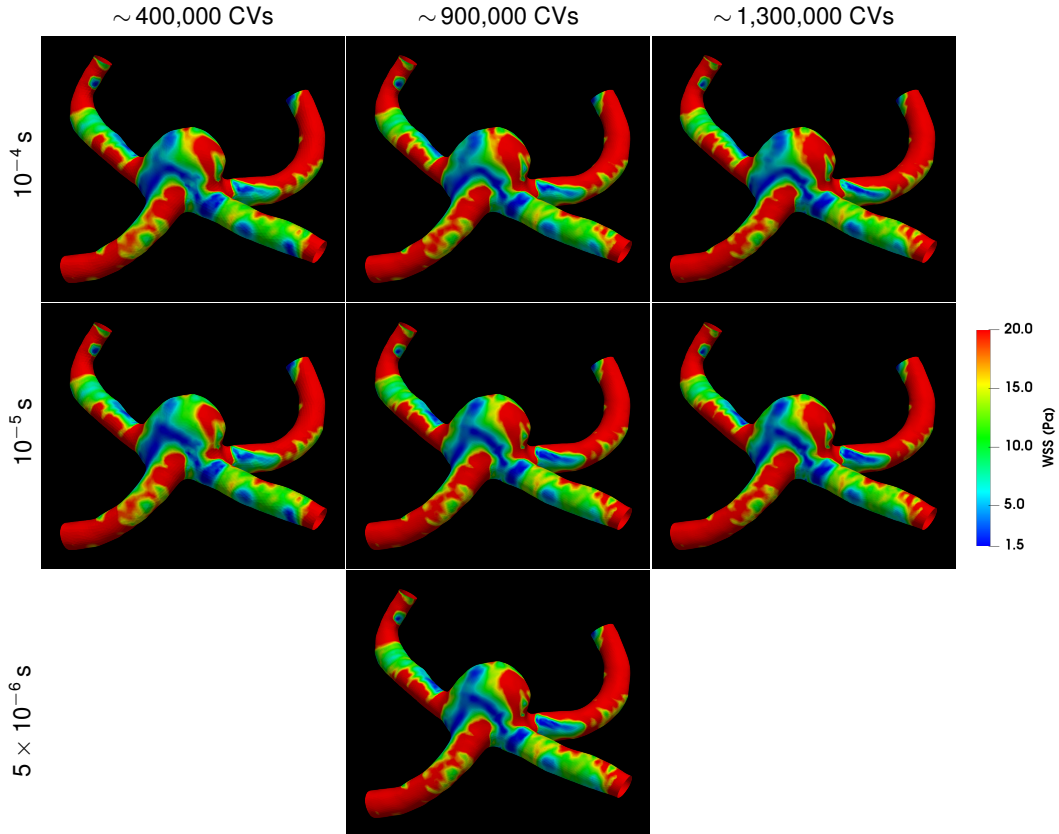
Thus, combining the results of WSS field and area-averaged WSS, we consider acceptable to adopt $\sim 850,000$ control volumes and 10^{-5} s for this geometry.

A.3 Case 17

Post-stent

Figure 33 shows the WSS field on the post-stent surface of case 17 for meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,300,000$ control volumes and time-steps of 10^{-4} , 10^{-5} , and 5×10^{-6} s. In this case, a qualitative analysis reveals no considerable differences in the WSS field between all meshes and time-steps. Therefore, we evaluated both spatial and temporal resolutions by means of the area-averaged WSS, shown in Figure 34. Despite the similarities in the area-averaged WSS, we note that mesh and time-step independence are effectively reached for $\sim 900,000$ control volumes and 10^{-5} s, respectively.

Figure 33 – Mesh and time-step independence analysis for the post-stent geometry of case 17: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,300,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.

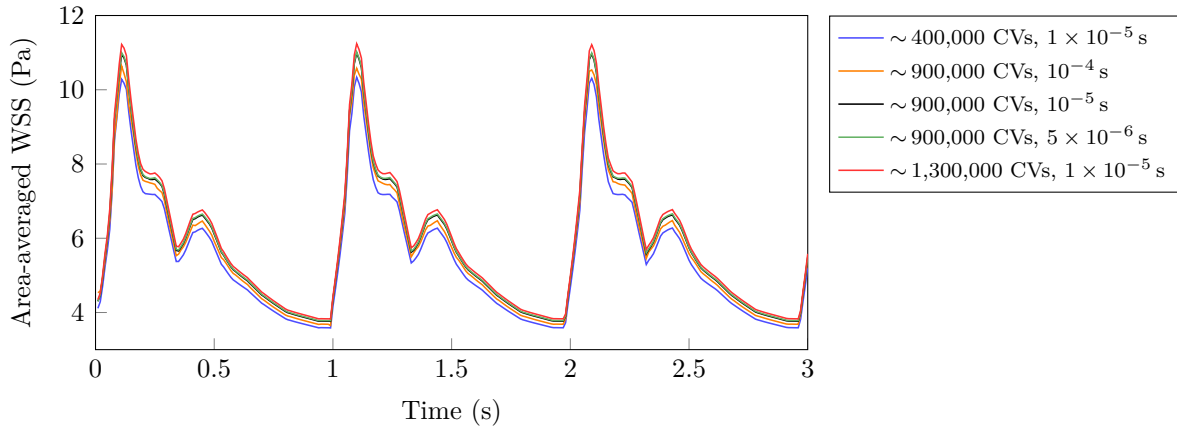


Source: prepared by the author.

Pre-stent

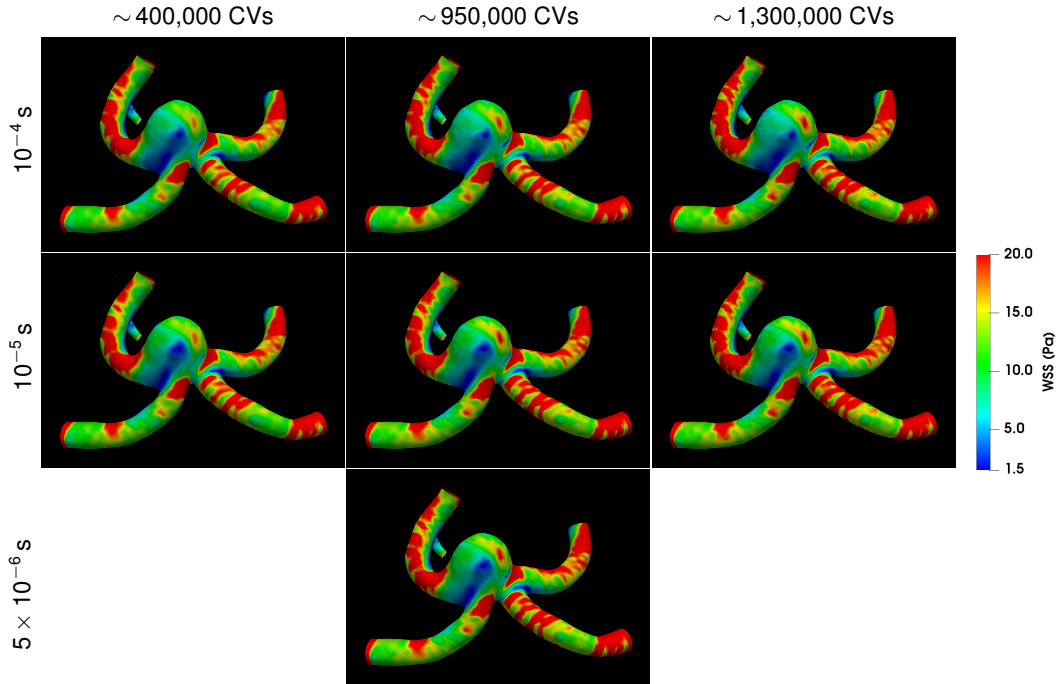
As for the pre-stent geometry of case 17, we note the same behavior from the post-stent geometry when comparing the WSS field for different meshes and time-steps (Figure 35). To come to a conclusion, we evaluated the area-averaged WSS for these meshes and time-

Figure 34 – Area-averaged WSS on the post-stent surface of case 17 as a function of time for different combinations of mesh and time-step resolution.



Source: prepared by the author.

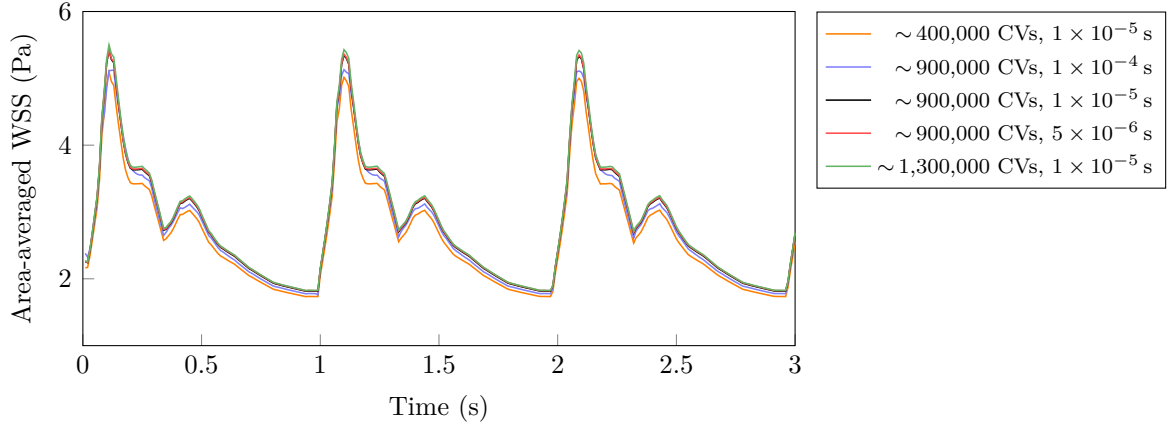
Figure 35 – Mesh and time-step independence analysis for the pre-stent geometry of case 17: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 950,000$, and $\sim 1,300,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.



Source: prepared by the author.

steps (Figure 36). Although the profiles present a good agreement, mesh and time-step independence are reached for $\sim 950,000$ control volumes and 10^{-5} s.

Figure 36 – Area-averaged WSS on the pre-stent surface of case 17 as a function of time for different combinations of mesh and time-step resolution.



Source: prepared by the author.

A.4 Case E1

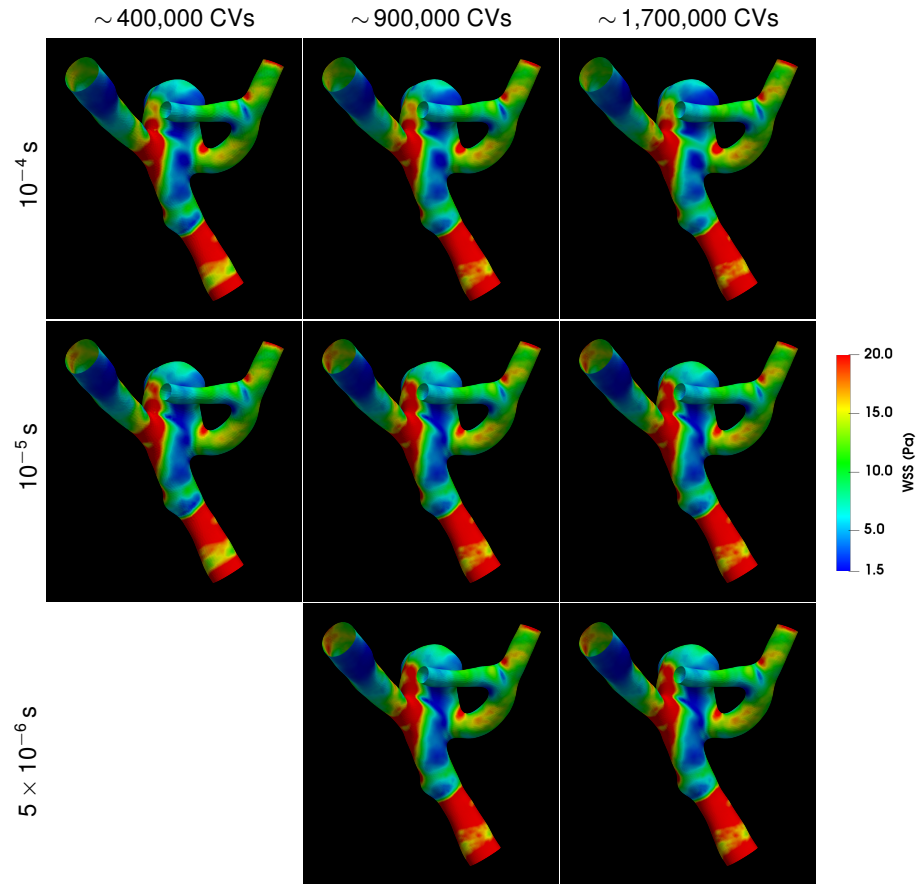
Post-stent

Figure 37 shows the WSS field on the post-stent surface of case E1 for meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s. A comparison between time-steps 10^{-4} s and 10^{-5} s reveals small differences in the WSS field; whereas comparing time-steps 10^{-5} s and 5×10^{-6} s no differences in the WSS field are noted, indicating independence of the temporal discretization for a time-step of 10^{-5} s. Regarding spatial resolution, we compared the area-averaged WSS for the three mesh sizes with a time-step of 10^{-5} s, shown in Figure 38. We note the two higher-order meshes in very close agreement, indicating that $\sim 900,000$ control volumes and a time-step of 10^{-5} s are able to represent the blood flow pattern in this geometry.

Pre-stent

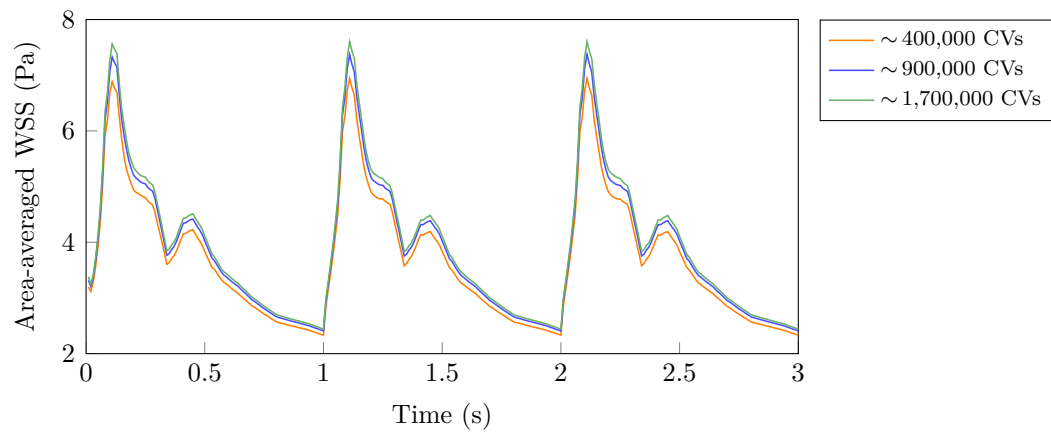
For the pre-stent geometry of case E1, Figure 39 shows the WSS field on mesh surfaces with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s. Once again, a comparison of the WSS field between the different time-steps reveals independence of the temporal discretization for a time-step of 10^{-5} s. For the spatial resolution, Figure 40 shows the area-averaged WSS for the three mesh sizes with a time-step 10^{-5} s. Once more, the two higher-order meshes present a similar profile, indicating that a mesh size of $\sim 900,000$ control volumes and a time-step of 5×10^{-5} are adequate to represent the blood flow in this geometry.

Figure 37 – Mesh and time-step independence analysis for the post-stent geometry of case E1: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.



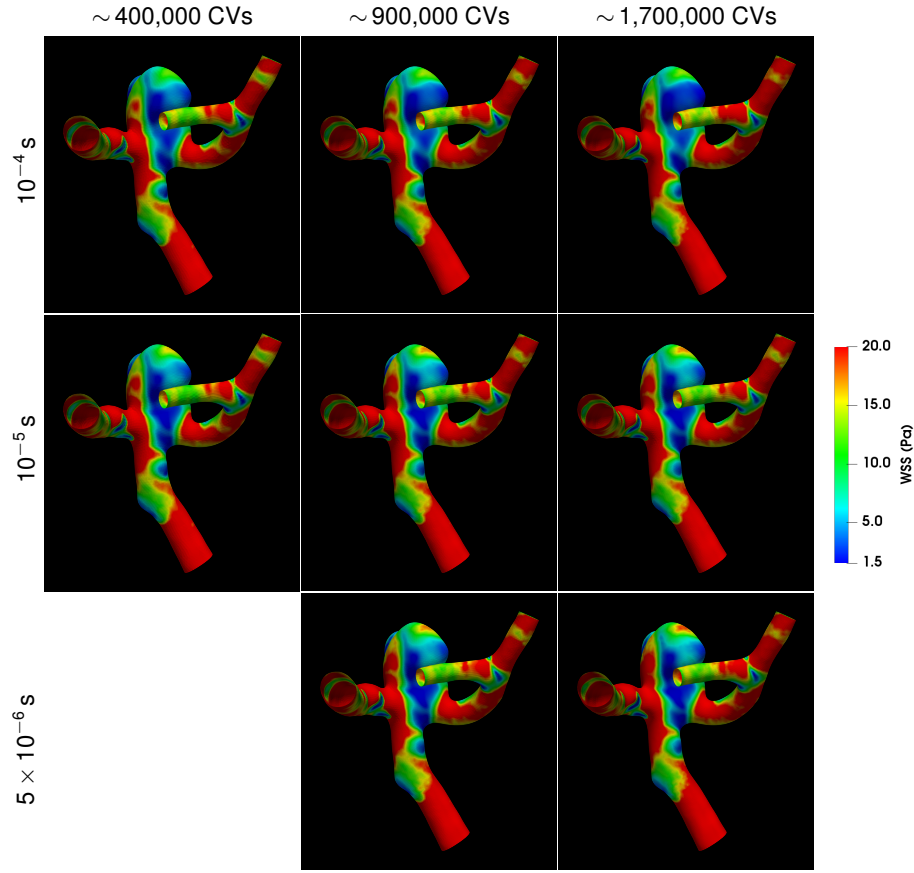
Source: prepared by the author.

Figure 38 – Area-averaged WSS on the post-stent surface of case E1 as a function of time for meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-5} s.



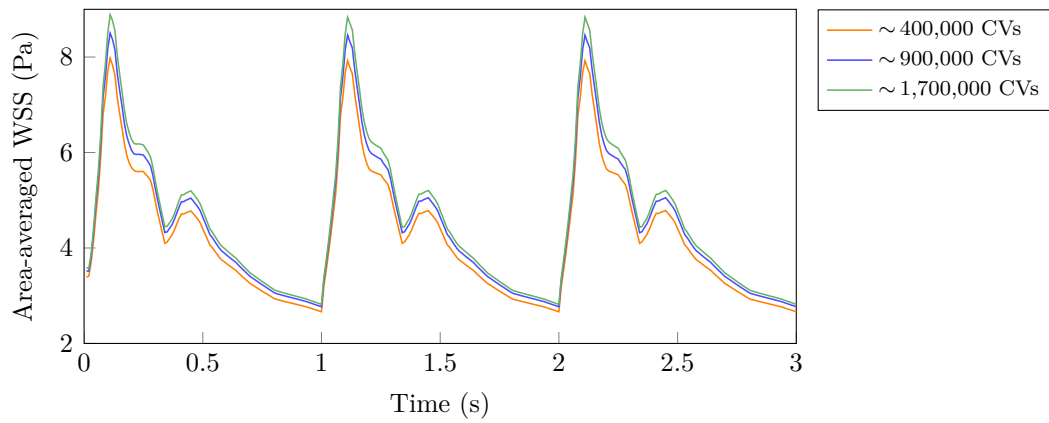
Source: prepared by the author.

Figure 39 – Mesh and time-step independence analysis for the pre-stent geometry of case E1: WSS field on surfaces of meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-4} s, 10^{-5} s, and 5×10^{-6} s.



Source: prepared by the author.

Figure 40 – Area-averaged WSS on the pre-stent surface of case E1 as a function of time for meshes with $\sim 400,000$, $\sim 900,000$, and $\sim 1,700,000$ control volumes and time-steps of 10^{-5} s.



Source: prepared by the author.

A.5 Final considerations

In recent years, the number of publications using computational methodologies to investigate hemodynamics in aneurysms has increased exponentially. However, often simulations are conducted and presented with computational efforts that do not do justice to the complexity of the fluid dynamics involved in aneurysm flows [60], as pointed out by recent studies [59, 61, 62].

For the cases studied here, we showed that a mesh size of $\sim 800,000$ tetrahedral control volumes and a time-step of 10^{-5} s are able to represent hemodynamic parameters of interest within an acceptable range of accuracy. Furthermore, these results are in close agreement with the recommendations of Hodis et al. [59] and Khan, Valen-Sendstad, and Steinman [62], who studied spatial and temporal resolutions for the blood flow in aneurysms. Despite arriving at similar results to those found in the literature, we agree with the assertion of Hodis et al. [59] that “each patient-specific model requires its own grid convergence study to establish the accuracy of the solution, because of the unique flow behavior generated by the geometric features of the anatomy”.

B – THE FINITE VOLUME DISCRETIZATION

We present here the Finite Volume Method (FVM) discretization procedure, which includes: modeling of the geometric domain and physical phenomena of interest; discretization of the geometric domain into a spatial mesh; discretization of the partial differential equations governing the physical problem into a system of algebraic equations; and solution of the resulting set of algebraic equations using an iterative process [43].

For that, we consider a flow domain Ω with velocity field $\mathbf{v}$ and fluid density ρ , where the conservation equation for a generic intensive quantity ϕ can be expressed as

$$\underbrace{\frac{\partial(\rho\mathbf{v})}{\partial t}}_{\text{temporal term}} + \underbrace{\nabla \cdot (\rho\mathbf{v}\phi)}_{\text{advective term}} = \underbrace{\nabla \cdot (I^\phi \nabla \phi)}_{\text{diffusive term}} + \underbrace{S^\phi}_{\text{source term}}, \quad (\text{B.1})$$

where I^ϕ is the diffusivity of ϕ . We assume that both $\mathbf{v}$ and ρ are known.

Let us consider that the flow domain Ω is now discretized into a finite number of non-overlapping elements—or control volumes—of arbitrary polyhedral shape, in a way that two neighboring elements must share only one face. For a cell-centered arrangement, the variables are stored at the centroid of the element, which is obtained as follows:

$$\mathbf{x}_c = \frac{1}{V_C} \int_{V_C} \mathbf{x} \, dV, \quad (\text{B.2})$$

where V_C is the total volume of the element.

Figure 41 shows a schematic finite volume mesh and also defines two geometric entities used in the FVM: the unit normal vector, $\mathbf{n}_f$, pointing outwards the element, and the vector joining the centroids of two neighboring elements, $\mathbf{d}_{cf}$.

Integrating Equation B.1 over the element V_C shown in Figure 41, we obtain

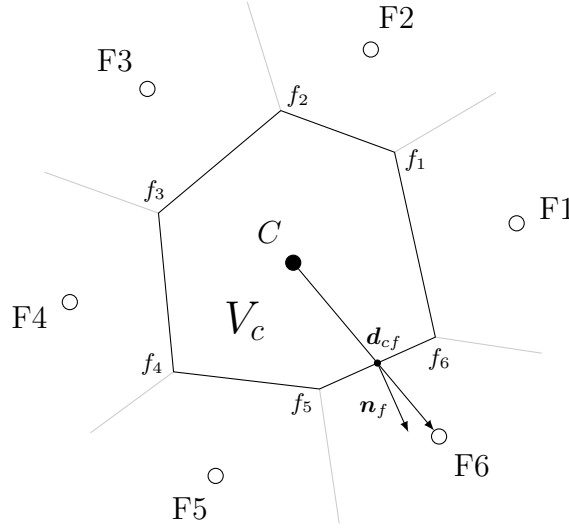
$$\int_{V_C} \frac{\partial(\rho\phi)}{\partial t} \, dV + \int_{V_C} \nabla \cdot (\rho\mathbf{v}\phi) \, dV = \int_{V_C} \nabla \cdot (I^\phi \nabla \phi) \, dV + \int_{V_C} S^\phi \, dV. \quad (\text{B.3})$$

Since the volume of the elements do not change with time, we can rewrite the above equation as

$$\frac{\partial}{\partial t} \int_{V_C} (\rho\phi) \, dV + \int_{V_C} \nabla \cdot (\rho\mathbf{v}\phi) \, dV = \int_{V_C} \nabla \cdot (I^\phi \nabla \phi) \, dV + \int_{V_C} S^\phi \, dV \quad (\text{B.4})$$

and make use of the Gauss' divergence theorem to replace the volume integrals of the

Figure 41 – Arbitrary polygonal element of a finite volume mesh, and its neighboring elements.



Source: prepared by the author.

advective and diffusive terms by surface integrals over the element surface, S_C , as follows:

$$\frac{\partial}{\partial t} \int_{V_C} (\rho\phi) dV + \oint_{S_C} (\rho\mathbf{v}\phi) \cdot \mathbf{n} dS = \oint_{S_C} (\Gamma^\phi \nabla \phi) \cdot \mathbf{n} dS + \int_{V_C} S^\phi dV, \quad (\text{B.5})$$

where $\mathbf{n}$ is the unit normal vector pointing outwards surface S_C . Furthermore, we replace the surface integrals over surface S_C by a sum of integrals over each face of the element V_C , yielding

$$\frac{\partial}{\partial t} \int_{V_C} (\rho\phi) dV + \sum_{f \sim \text{nb}(C)} \left[\int_{S_f} (\rho\mathbf{v}\phi) \cdot \mathbf{n} dS \right] = \sum_{f \sim \text{nb}(C)} \left[\int_{S_f} (\Gamma^\phi \nabla \phi) \cdot \mathbf{n} dS \right] + \int_{V_C} S^\phi dV, \quad (\text{B.6})$$

where $f \sim \text{nb}(C)$ refers to the faces of element V_C and S_f to their area.

To proceed further with the discretization, we need to evaluate the surface integrals at each face of element V_C ; this is done using a Gaussian quadrature. The process involves selection of integration points, which influences directly both the accuracy and computational cost. A common approach in the FVM adopts one integration point at the face centroid, which is a simple mean value integration and therefore, second order accurate [43].

As for the generic intensive quantity ϕ , we assume a linear variation within element V_C , i.e., $\phi = \phi(\mathbf{x})$, yielding

$$\phi(\mathbf{x}) = \phi_C + (\mathbf{x} - \mathbf{x}_C) \cdot (\nabla \phi)_C, \quad (\text{B.7})$$

where $\phi_C = \phi(\mathbf{x}_C)$. This linear function is also second order accurate, which can be verified writing the Taylor series expansion of ϕ around point C :

$$\begin{aligned} \phi(\mathbf{x}) = & \phi(\mathbf{x}_C) + (\mathbf{x} - \mathbf{x}_C) \cdot (\nabla \phi)_C + \frac{1}{2!} (\mathbf{x} - \mathbf{x}_C)^2 : (\nabla \nabla \phi)_C \\ & + \frac{1}{3!} (\mathbf{x} - \mathbf{x}_C)^3 :: (\nabla \nabla \nabla \phi)_C + \dots \dots \dots \\ & + \frac{1}{n!} (\mathbf{x} - \mathbf{x}_C)^n \underbrace{:: \dots ::}_{(n-1) \text{ times}} \left(\underbrace{\nabla \nabla \dots \nabla}_{n \text{ times}} \phi \right)_C + \dots \dots \dots, \end{aligned} \quad (\text{B.8})$$

where $(\mathbf{x} - \mathbf{x}_C)^n$ represents the n^{th} tensorial product of the vector $(\mathbf{x} - \mathbf{x}_C)$ with itself, resulting a n^{th} rank tensor. The operator “:” is the inner product of two second rank tensors, and more generally “ $\underbrace{:: \dots ::}_{(n-1) \text{ times}}$ ” is the inner product of two n^{th} rank tensors, both yielding a scalar. Comparing Equations B.7 and B.8, we conclude that the error is proportional to $|(\mathbf{x} - \mathbf{x}_C)^2|$.

Finally, introducing Equation B.7 into Equation B.6, yields

$$\frac{\partial}{\partial t} \int_{V_C} (\rho \phi) dV + \sum_{f \sim \text{nb}(C)} [\rho_f (\mathbf{v}_f \cdot \mathbf{s}_f)] \phi_f = \sum_{f \sim \text{nb}(C)} (\rho \Gamma^\phi)_f (\nabla \phi_f) \cdot \mathbf{s}_f + \int_{V_C} S^\phi dV, \quad (\text{B.9})$$

where the lower index f indicates a variable evaluated at the face centroid. Now, we must interpolate the variables ϕ_f and $\nabla \phi_f$ at face centroid from neighboring cell centroid variables, which are presented next.

B.1 Spatial discretization

Advective term

The advective term is expressed as

$$\sum_{f \sim \text{nb}(C)} [\rho_f (\mathbf{v}_f \cdot \mathbf{s}_f)] \phi_f, \quad (\text{B.10})$$

where $\rho_f (\mathbf{v}_f \cdot \mathbf{s}_f) = \dot{m}_f$ is the mass flow rate through face f . At this point, the FVM evaluates the mass flow rate interpolating ρ_f explicitly, i.e., using known values from previous iterations. For the incompressible case, ρ is constant within the entire fluid domain and thus, known at face centroids. On the other hand, ϕ_f is evaluated implicitly, i.e., it is interpolated from values of the same iteration at adjacent cell centroids— ϕ_C and ϕ_F .

Regarding the interpolation of ϕ_f , it must be chosen carefully in order to avoid unnatural behavior of the solution. For example, first-order schemes introduce numerical diffusion into the solution; second-order schemes can cause “wiggles” in decelerating

flows and lead to non-physical solutions [41, 43]. Therefore, higher order schemes are normally recommended. For the flow in aneurysms, we adopted a linear, upwind-biased scheme, which is second-order accurate but presents far less numerical dispersion than other second-order schemes. For unstructured meshes, ϕ_f can be expressed as

$$\phi_f = \phi_C + (2\nabla\phi_C - \nabla\phi_f) \cdot \mathbf{d}_{Cf}, \quad (\text{B.11})$$

where $\mathbf{d}_{Cf} = (\mathbf{x}_C - \mathbf{x}_f)$ is the vector joining cell centroid C and face f . As for the gradients in Equation B.11, we will discuss them later.

Finally, applying the interpolation scheme for ϕ_f , it can be written as

$$\phi_f = w\phi_C + (1-w)\phi_F = \phi_F + w(\phi_C - \phi_F), \quad (\text{B.12})$$

where w is a weight that depends on the selected interpolation scheme and accounts for the influence of ϕ_C and ϕ_F over ϕ_f .

Diffusive term

The diffusive term is represented by

$$\sum_{f \sim \text{nb}(C)} \left(\rho \Gamma^\phi \right)_f (\nabla \phi_f) \cdot \mathbf{s}_f. \quad (\text{B.13})$$

First, we need to evaluate the fluid density and diffusivity of ϕ . A simple approach uses the assumption of linear variation of these properties between centroids C and F . Therefore,

$$\rho_f = g_C \rho_C + (1 - g_C) \rho_F \quad \text{and} \quad \Gamma_f^\phi = g_C \Gamma_C^\phi + (1 - g_C) \Gamma_F^\phi,$$

where g_C is an integration factor in terms of distances between cell and face centroids given by

$$g_C = \frac{\|\mathbf{r}_F - \mathbf{r}_f\|}{\|\mathbf{r}_F - \mathbf{r}_C\|} = \frac{d_{Ff}}{d_{CF}}. \quad (\text{B.14})$$

Note that this is a general approach for evaluating these properties at face centroids. For incompressible flows, for example, the density is constant all over the fluid domain and thus, already known.

The gradient of ϕ normal to face f , $(\nabla \phi_f) \cdot \mathbf{s}_f$, can be expressed in terms of a directional derivative in the direction normal to the face f as follows:

$$(\nabla \phi_f) \cdot \mathbf{s}_f = (\nabla \phi_f) \cdot (S_f \mathbf{n}) = S_f \left(\frac{\partial \phi}{\partial \mathbf{n}} \right)_f, \quad (\text{B.15})$$

where $\mathbf{s}_f = \mathbf{n}S_f$, with $\mathbf{n}$ being the unit normal vector to the surface and S_f the surface area. For structured meshes, $\mathbf{n}$ lays in the direction defined by the line connecting centroids C and F ; therefore, the directional derivative can be evaluated with second-order accuracy, using the Central Differences scheme, yielding

$$\left(\frac{\partial \phi}{\partial \mathbf{n}}\right)_f = \frac{\phi_F - \phi_C}{\|\mathbf{r}_F - \mathbf{r}_C\|} = \frac{\phi_F - \phi_C}{d_{CF}}. \quad (\text{B.16})$$

However, for unstructured meshes, we cannot ensure that $\mathbf{n}$ and $\mathbf{d}_{CF}$ are collinear—see Figure 41. To address this problem, we write $\mathbf{s}_f$ as a sum of two vectors, i.e.,

$$\mathbf{s}_f = \mathbf{E}_f + \mathbf{T}_f \quad (\text{B.17})$$

with $\mathbf{E}_f$ being in the $\mathbf{d}_{CF}$ direction, which enables writing part of the diffusion flux as a function of nodal values ϕ_F and ϕ_C using a Central Differences scheme [43] such that

$$\begin{aligned} (\nabla \phi_f) \cdot \mathbf{s}_f &= \underbrace{(\nabla \phi_f) \cdot \mathbf{E}_f}_{\text{orthogonal contribution}} + \underbrace{(\nabla \phi_f) \cdot \mathbf{T}_f}_{\text{non-orthogonal contribution}} \\ &= E_f \frac{\phi_F - \phi_C}{d_{CF}} + (\nabla \phi_f) \cdot \mathbf{T}_f. \end{aligned} \quad (\text{B.18})$$

The second term on the right-hand side is called cross-diffusion and appears as a result of the mesh non-orthogonality. To evaluate $\mathbf{T}_f$, OpenFOAM uses a over-relaxed approach, in which the importance of the orthogonal term is intensified as the mesh non-orthogonality increases. This is achieved by selecting $\mathbf{T}_f$ to be normal to $\mathbf{s}_f$, as shown in Figure 42. Mathematically, $\mathbf{T}_f = \mathbf{s}_f - \mathbf{E}_f$, with

$$\mathbf{E}_f = E_f \mathbf{e} = \left(\frac{\mathbf{s}_f}{\cos \theta} \right) \mathbf{e} = \left(\frac{S_f^2}{S_f \cos \theta} \right) \mathbf{e} = \frac{\mathbf{s}_f \cdot \mathbf{s}_f}{\mathbf{e} \cdot \mathbf{s}_f} \mathbf{e} \quad (\text{B.19})$$

and thus, resulting in

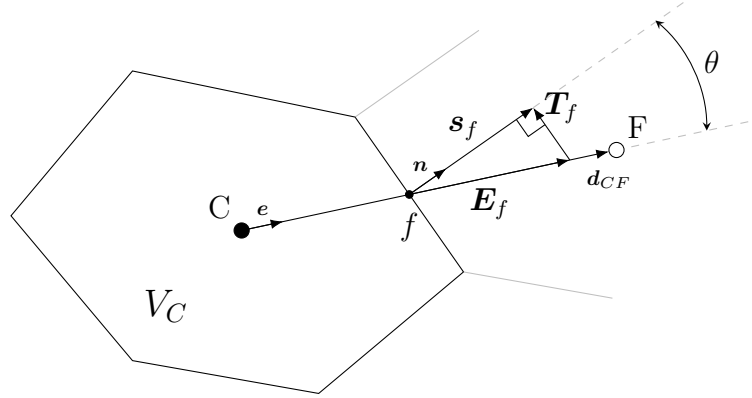
$$(\nabla \phi_f) \cdot \mathbf{s}_f = \underbrace{E_f \frac{\phi_F - \phi_C}{d_{CF}}}_{\text{orthogonal-like term}} + \underbrace{(\nabla \phi_f) \cdot \left(\mathbf{n} - \frac{\mathbf{e}}{\cos \theta} \right) S_f}_{\text{cross-diffusion term}}. \quad (\text{B.20})$$

Note that the cross-diffusion term cannot be expressed in terms of nodal values; therefore, it is evaluated in a deferred manner, using the current gradient field and adding it as a source to the right-hand side of the resulting algebraic equation [43].

Gradient discretization

As already discussed above, we must evaluate the gradients at cell centroid, $\nabla \phi_C$, and at face centroids, $\nabla \phi_f$. OpenFOAM offers different techniques for gradient discretization,

Figure 42 – Over-relaxed decomposition of the normal surface vector $\mathbf{s}_f$. $\mathbf{E}_f$ lays in the $\mathbf{d}_{CF}$ direction and $\mathbf{T}_f$ is normal to $\mathbf{s}_f$.



Source: prepared by the author.

such as the standard Green-Gauss method, the second-order least square method, and the forth-order least square method. We present here the Green-Gauss method. For that, we make use of the mean value theorem to express the gradient as follows:

$$\nabla\phi_C = \frac{1}{V_C} \int_{V_C} \nabla\phi \, dV. \quad (\text{B.21})$$

Then, we use a variant of Gauss' divergence theorem to transform the volume integral into a surface integral over the surface S_C of the control volume V_C :

$$\int_{V_C} \nabla\phi \, dV = \oint_{S_C} \phi \mathbf{n} \, dV. \quad (\text{B.22})$$

And as already shown previously, we are able to express surface integrals as a sum of integrals, which in turn can be approximated using a linear Gaussian quadrature over the element face, yielding

$$\nabla\phi_C = \frac{1}{V_C} \sum_{f \sim \text{nb}(C)} \phi_f \mathbf{s}_f. \quad (\text{B.23})$$

As for the gradients at face centroids, $\nabla\phi_f$, they are linearly interpolated from the nodes straddling the face, using a stencil heavily based on cell centroids straddling the face, which is given by

$$\nabla\phi_f = \overline{\nabla\phi_f} + \underbrace{\left[\frac{\phi_F - \phi_C}{d_{CF}} - \overline{\nabla\phi_f} \cdot \mathbf{d}_{CF} \right] \mathbf{d}_{CF}}_{\text{correction term}} \quad (\text{B.24})$$

with $\overline{\nabla\phi_f} = g_C \nabla\phi_C + (1 - g_C) \nabla\phi_F$.

Source terms

Using the mean value theorem, we can express the source term as follows:

$$\int_{V_C} S^\phi dV = S_C^\phi V_C, \quad (\text{B.25})$$

where S_C^ϕ is, in general, a function of the variable ϕ and thus, can be expressed as $S_C^\phi = S(\phi_C)$. However, the form of the source term function is particular to each differential equation. Therefore, further discretization depends on the differential equation. For constant or relatively small values, S_C^ϕ can be calculated explicitly using available values of ϕ from previous iterations.

B.2 Temporal discretization

By now, the discretization procedure enabled us to write all non-transient terms—advective, diffusive, and source terms—as functions of nodal values of the generic intensive quantity ϕ . Thus, we can rewrite the transport equation into a more compact form using a spatial operator that includes all non-transient terms as follows:

$$\frac{\partial(\rho\phi)}{\partial t} + \mathcal{L}(\phi) = 0, \quad (\text{B.26})$$

where

$$\mathcal{L}(\phi) = \nabla \cdot (\rho \mathbf{v} \phi) - \nabla \cdot (\Gamma^\phi \nabla \phi) - S^\phi. \quad (\text{B.27})$$

Integrating the transport equation over a control volume V_C and applying the spatial discretization about the cell centroids yields:

$$\frac{\partial(\rho\phi_C)}{\partial t} V_C + \mathcal{L}[\phi_C(t)] = 0, \quad (\text{B.28})$$

where $\phi_C(t)$ represents the nodal values expressed at a time-level t .

The discretization of the transient term is based on the Finite Differences Method, using a second-order Euler backward scheme. Therefore, we use a Taylor series expansion to express $\phi = \phi(t)$ around time-levels $(t - \Delta t)$ and $(t - 2\Delta t)$, i.e.,

$$\Phi_C(t - \Delta t) = \Phi_C(t) - \frac{\partial \Phi_C}{\partial t}(t) \Delta t + \frac{1}{2!} \frac{\partial^2 \Phi_C}{\partial^2 t}(t) (\Delta t)^2 + \mathcal{O}(\Delta t^3)$$

and

$$\Phi_C(t - 2\Delta t) = \Phi_C(t) - \frac{\partial \Phi_C}{\partial t}(t) (2\Delta t) + \frac{1}{2!} \frac{\partial^2 \Phi_C}{\partial^2 t}(t) (2\Delta t)^2 + \mathcal{O}(\Delta t^3),$$

where $\Phi_C = \rho_C \phi_C$. Multiplying the first equation by four and subtracting the second from it, we are able to eliminate the second and higher-order derivatives, yielding

$$\begin{aligned} 4\Phi_C(t - \Delta t) - \Phi_C(t - 2\Delta t) &= 3\Phi_C(t) - 2\frac{\partial\Phi_C}{\partial t}(t)\Delta t + \mathcal{O}(\Delta t^3) \implies \\ \implies \frac{\partial\Phi_C}{\partial t}(t) &= \frac{3\Phi_C(t) - 4\Phi_C(t - \Delta t) + \Phi_C(t - 2\Delta t)}{2\Delta t} + \mathcal{O}(\Delta t^3). \end{aligned} \quad (\text{B.29})$$

And substituting back into Equation B.28 yields

$$\left(\frac{3\Phi_C(t) - 4\Phi_C(t - \Delta t) + \Phi_C(t - 2\Delta t)}{2\Delta t} \right) V_C + \mathcal{L}[(\phi_C(t))] = 0. \quad (\text{B.30})$$

Denoting time-levels by a superscript n and substituting back $\Phi_C = \rho_C \phi_C$, the last equation is rewritten as

$$\left(\frac{3\rho_C^n \phi_C^n - 4\rho_C^{n-1} \phi_C^{n-1} + \rho_C^{n-2} \phi_C^{n-2}}{2\Delta t} \right) V_C + \mathcal{L}[\phi_C^n] = 0. \quad (\text{B.31})$$

Substituting back Equations B.12, B.16 and B.27 into the last equation yields a linearized equation for the control volume V_C as follows:

$$\begin{aligned} \left(\frac{3\rho_C^n \phi_C^n - 4\rho_C^{n-1} \phi_C^{n-1} + \rho_C^{n-2} \phi_C^{n-2}}{2\Delta t} \right) V_C + \sum_{f \sim \text{nb}(C)} \overbrace{[\rho_f(\mathbf{v}_f \cdot \mathbf{s}_f)]}^{\dot{m}_f} [w\phi_C^n + (1-w)\phi_F^n] = \\ = \sum_{f \sim \text{nb}(C)} \left(\rho \Gamma^\phi \right)_f \left[\frac{E_f}{d_{CF}} (\phi_F^n - \phi_C^n) + \nabla \phi_f \cdot \mathbf{T}_f \right] + V_C (S_C^\phi)^{n-1}. \end{aligned} \quad (\text{B.32})$$

Grouping similar terms, we obtain an algebraic linearized equation for the control volume V_C :

$$a_C \phi_C^n + \sum_{F \sim \text{NB}(C)} a_F^\phi \phi_F^n = b_C^\phi, \quad (\text{B.33})$$

where $F \sim \text{NB}(C)$ represents cell centroids neighboring the control volume V_C and the coefficients a_C^ϕ , a_F^ϕ , and b_C^ϕ are given by

$$\begin{aligned} a_C^\phi &= \frac{3\rho_C V_C}{2\Delta t} + \sum_{f \sim \text{nb}(C)} \left(w\dot{m}_f + \rho_f \Gamma_f^\phi \frac{E_f}{d_{CF}} \right), \\ a_F^\phi &= (1-w)\dot{m}_f - \rho_f \Gamma_f^\phi \frac{E_f}{d_{CF}}, \text{ and} \\ b_C^\phi &= V_C (S_C^\phi)^n + \sum_{f \sim \text{nb}(C)} \rho_f \Gamma_f^\phi \nabla \phi_f \cdot \mathbf{T}_f + \frac{4\rho_C^{n-1} \phi_C^{n-1} V_C}{2\Delta t} - \frac{\rho_C^{n-2} \phi_C^{n-2} V_C}{2\Delta t}. \end{aligned} \quad (\text{B.34})$$

Equation B.33 represents an algebraic linearized equation for one control volume in a finite volume mesh. Considering all control volumes in a mesh, we are able to assemble a linear system of algebraic equations as follows:

$$\mathbf{A}^\phi \boldsymbol{\phi} = \mathbf{b}^\phi, \quad (\text{B.35})$$

where $\mathbf{A} \in \mathbb{R}^{N_{CV} \times N_{CV}}$ represents the matrix of coefficients: a_C^ϕ occupying the diagonal and a_F^ϕ occupying other positions in the line; N_{CF} is the total number of control volumes in the mesh; $\mathbf{b}^\phi \in \mathbb{R}^{N_{CV}}$ is the source coefficients vector; and $\boldsymbol{\phi} \in \mathbb{R}^{N_{CV}}$ is the solution vector. A schematic representation of the assembled linear system of algebraic equations is presented in Figure 43.

Figure 43 – Schematic representation of the assembled linear system of algebraic equations: a_C^ϕ coefficients are found at the matrix diagonal and a_F^ϕ coefficients occupy other positions in the line.

$$\begin{bmatrix}
 \bullet & & & & \circ & \circ & \circ & & \\
 & \bullet & & & \circ & & & \circ & \\
 \circ & \circ & \bullet & & & & & \circ & \circ \\
 & & & \bullet & & \circ & & & \\
 & & & & \bullet & \circ & \circ & \circ & \circ \\
 \circ & \circ & & & \bullet & & \circ & & \\
 & & & & & & & & \\
 a_{F1} & & a_{F2} & & a_C & & a_{F3} & &
 \end{bmatrix}
 \begin{bmatrix}
 \phi_C
 \end{bmatrix}
 =
 \begin{bmatrix}
 b_C
 \end{bmatrix}$$

Source: prepared by the author.

To complete our discretization, we must discretize the boundary conditions. However, each type of boundary conditions has a specific discretization procedure; thus, we recommend the writings of Moukalled, Mangani, and Darwish [43] for more details on the discretization of boundary conditions. Also, note that the assembled linear system, Equation B.35, represents the spatial discretization of the transport equation of a generic intensive quantity ϕ in a flow domain Ω at one time-step. In order to solve the problem in a time-marching manner, the system must be solved for each time-step.

B.3 Pressure-velocity coupling

So far, we presented a procedure for discretizing the transport equation for a generic intensive variable ϕ in a flow domain with known velocity field $\mathbf{v}$ —Equation B.1. For the fluid flow phenomena, we can reform the general transport equation into the continuity and momentum equations. Considering an incompressible Newtonian fluid with constant density ρ and dynamic viscosity μ , this system of partial differential equations is known as Navier-Stokes equations:

$$\nabla \cdot (\rho \mathbf{v}) = 0 \quad (\text{B.36})$$

and

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot [\mu(\nabla \mathbf{v} + \nabla^T \mathbf{v})] + \mathbf{f}_b, \quad (\text{B.37})$$

where p is the pressure field and $\mathbf{f}_b$ represent body forces acting on the flow.

Note that the set of Navier-Stokes equations have the pressure and velocity fields as unknowns. However, while the velocity field can be computed from the momentum equation, the pressure field cannot be directly computed from the continuity equation. This reveals an implicit coupling between pressure and velocity, what makes the solution of the Navier-Stokes equations by any iterative method unsustainable. Thereby, we must derive an equation for pressure and use algorithms that can deal with the pressure-velocity coupling. We present here two algorithms to solve the set of Navier-Stokes equations: the SIMPLE proposed by Patankar [63]; and the PISO proposed by Issa, Gosman, and Watkins [56].

SIMPLE algorithm

We first consider the discretized form of the continuity and momentum equations, respectively:

$$\sum_{f \sim \text{nb}(C)} \dot{m}_f = 0 \quad (\text{B.38})$$

and

$$a_C^v \mathbf{v}_C + \sum_{F \sim \text{NB}(C)} a_F^v \mathbf{v}_F = \mathbf{b}_C^v, \quad (\text{B.39})$$

where the coefficients, according to the discretization procedure presented before, are given by

$$\begin{aligned}
a_C^v &= \frac{3\rho_C^n V_C}{2\Delta t} + \sum_{f \sim \text{nb}(C)} \left(w \dot{m}_f + \mu_f \frac{E_f}{d_{CF}} \right), \\
a_F^v &= (1-w) \dot{m}_f - \mu_f \frac{E_f}{d_{CF}}, \text{ and} \\
\mathbf{b}_C^v &= (\mathbf{f}_b)_C V_C + \frac{4V_C}{2\Delta t} \rho_C^{n-1} \mathbf{v}_C^{n-1} - \frac{V_C}{2\Delta t} \rho_C^{n-2} \mathbf{v}_C^{n-2} + \sum_{f \sim \text{nb}(C)} \mu_f \nabla \mathbf{v}_f \cdot \mathbf{T}_f \\
&\quad - (\nabla p)_C V_C + \sum_{f \sim \text{nb}(C)} \mu_f \nabla^T \mathbf{v}_f \cdot \mathbf{s}_f
\end{aligned}$$

with $\dot{m}_f = \rho_f \mathbf{v}_f \cdot \mathbf{s}_f$ as the mass flow rate through cell faces, obtained using available values from the last iteration. Defining $\mathbf{b}_C^v = \tilde{\mathbf{b}}_C^v - (\nabla p)_C V_C$ and the following vector operators:

$$\begin{aligned}
\mathbf{H}_C[\mathbf{v}] &= \sum_{F \sim \text{NB}(C)} \frac{a_F^v}{a_C^v} \mathbf{v}_F, \\
\mathbf{B}_C^v &= \frac{\tilde{\mathbf{b}}_C^v}{a_C^v}, \text{ and} \\
\mathbf{D}_C^v &= \frac{V_C}{a_C^v};
\end{aligned}$$

the momentum equation can be written in a more compact and convenient form for future derivations:

$$\mathbf{v}_C + \mathbf{H}_C[\mathbf{v}] = -\mathbf{D}_C^v (\nabla p)_C + \mathbf{B}_C^v. \quad (\text{B.40})$$

It is important to note that the collocate FVM stores variables at cell centroids. Still, to evaluate $\dot{m}_f$, we need the velocities at cell centroids. An intuitive approach would be use a linear interpolation between cell centroids straddling the cell face. However, this has been proven to lead to the checkboard problem: a non-physical zigzag pressure and velocity fields. Rhie and Chow [55] proposed a solution, in which a pseudo-momentum equation is constructed at cell faces and then used to compute $\dot{m}_f$.

Finally, the SIMPLE algorithm comprises the following steps:

1. To calculate the solution at iteration $n + 1$, use the solution at previous iteration for the pressure and velocity fields, i.e., p^n and $\mathbf{v}^n$ and compute the mass flow rate at cell faces, $\dot{m}_f^n$;
2. Solve the momentum equation (Equation B.39) to obtain a new velocity field $\mathbf{v}_C^*$. Note that the new velocity field satisfies the momentum equation but does not necessarily

satisfy the continuity equation (Equation B.38). At this step, the momentum equation can be expressed as

$$\mathbf{v}_C^* + \mathbf{H}_C[\mathbf{v}^*] = -\mathbf{D}_C^v(\nabla p)_C + \mathbf{B}_C^v. \quad (\text{B.41})$$

3. Compute a momentum-satisfying mass flow rate $\dot{m}_f$ at cell faces using the Rhie-Chow interpolation, given by

$$\mathbf{v}_f^* = \overline{\mathbf{v}}_f^* - \overline{\mathbf{D}}_f^v \left(\nabla p_f^n - \overline{\nabla p}_f^n \right), \quad (\text{B.42})$$

where $\overline{\square}_f = g_C \square_C + (1 - g_C) \square_F$ represents a linear interpolation between cell centroids straddling face f , g_C is a geometric factor (Equation B.14), and ∇p_f is computed as presented in Equation B.24; therefore, yielding

$$\dot{m}_f = \rho_f \mathbf{v}_f^* \cdot \mathbf{s}_f = \rho_f \overline{\mathbf{v}}_f^* \cdot \mathbf{s}_f - \rho_f \overline{\mathbf{D}}_f^v \left(\nabla p_f^n - \overline{\nabla p}_f^n \right) \cdot \mathbf{s}_f, \quad (\text{B.43})$$

4. Once the new mass flow rate depends on the velocity field $\mathbf{v}^*$, it also does not necessarily satisfy the continuity equation. Thereby, a correction term $\dot{m}'_f$ is adopted so that

$$\dot{m}_f = \dot{m}_f^* + \dot{m}'_f \quad (\text{B.44})$$

and in a similar way, we define a correction velocity and pressure fields at cell centroids, respectively, as

$$\mathbf{v}_C = \mathbf{v}_C^* + \mathbf{v}'_C \quad \text{and} \quad p_C = p_C^n + p'_C.$$

Note that the mass flow rate $\dot{m}_f$ satisfies the continuity equation and therefore,

$$\sum_{f \sim \text{nb}(C)} \dot{m}_f = 0 \Rightarrow \sum_{f \sim \text{nb}(C)} \dot{m}'_f = - \sum_{f \sim \text{nb}(C)} \dot{m}_f^*. \quad (\text{B.45})$$

Using the corrected velocity field at face centroid $\mathbf{v}'_f$ calculated via Rhie-Chow interpolation from cell centroids $\mathbf{v}'_C$ and $\mathbf{v}'_F$ into the last equation leads to a pressure

correction equation, given by

$$\begin{aligned}
& \sum_{f \sim \text{nb}(C)} \rho_f \mathbf{v}'_f \cdot \mathbf{s}_f = - \sum_{f \sim \text{nb}(C)} \dot{m}_f^* \Rightarrow \\
& \Rightarrow \sum_{f \sim \text{nb}(C)} \rho_f \underbrace{\left[\overline{\mathbf{v}'_f} - \overline{\mathbf{D}_f^{\mathbf{v}'}}(\nabla p'_f) - \overline{\mathbf{D}_f^{\mathbf{v}'}}(\overline{\nabla p'_f}) \right]}_{-\overline{\mathbf{H}_f}[\mathbf{v}']} \cdot \mathbf{s}_f \Rightarrow \\
& \Rightarrow - \sum_{f \sim \text{nb}(C)} \rho_f \overline{\mathbf{D}_f^{\mathbf{v}'}}(\nabla p'_f) \cdot \mathbf{s}_f = - \sum_{f \sim \text{nb}(C)} \dot{m}_f^* + \underbrace{\sum_{f \sim \text{nb}(C)} \rho_f \overline{\mathbf{H}_f}[\mathbf{v}'] \cdot \mathbf{s}_f}_{\text{neglected}}.
\end{aligned} \tag{B.46}$$

In the SIMPLE algorithm, the underlined term is neglected, thus linking the velocity correction field directly to pressure corrections. After discretizing the surface normal pressure gradient, the last equation can be expressed as

$$a_C^{p'} p'_C + \sum_{F \sim \text{NB}(C)} a_F^{p'} p'_F = b_C^{p'}, \tag{B.47}$$

which represents an algebraic equation for the pressure correction at the centroid of one control volume V_C . Assembling for the whole mesh and solving the linear system yields a velocity correction,

$$\mathbf{v}'_C = -\mathbf{D}_C^v \nabla p'_C. \tag{B.48}$$

5. After computing the pressure correction field, correct velocity and pressure fields at cell centroids and mass flow rate at face centroids to obtain continuity-satisfying fields.

$$\begin{aligned}
\mathbf{v}_C^{**} &= \mathbf{v}_C^* + \mathbf{v}'_C, \\
\dot{m}_f^{**} &= \dot{m}_f^* + \dot{m}'_f = \dot{m}_f^{**} - \rho_f \overline{\mathbf{D}_f^v} \nabla p'_f \cdot \mathbf{s}_f, \text{ and} \\
p_C^* &= p_C^n + \lambda^p p'_C,
\end{aligned} \tag{B.49}$$

where λ^p is an under relaxation factor used to increase robustness and improve the convergence behavior;

6. Use the new velocity and pressure fields and mass flow rate as initial guess. Return to step 2 and repeat until convergence;
7. Set the solution at time $n + 1$ (or $t + \Delta t$) to be equal to the converged solution and set $n \leftarrow n + 1$;
8. Advance to the next time-step, return to step 1, and repeat until the last time-step.

PISO algorithm

The PISO algorithm [56] is one of the most adopted variants of the SIMPLE algorithm. In this variant, the $\mathbf{H}[\mathbf{v}']$ is no longer neglected; instead it is used as part of the correction procedure composed of two more steps. The PISO correction loop takes place between steps 6 and 7 of the SIMPLE algorithm and comprises the following steps.

1. Using the corrected pressure and velocity fields and the corrected mass flow rate, i.e., $\mathbf{v}^{**}$, p^* , and $\dot{m}^{**}$, update the momentum equation and solve explicitly for $\mathbf{v}^{***}$:

$$\mathbf{v}_C^{***} = -\mathbf{H}^{**}[\mathbf{v}_C^{**}] - (\mathbf{D}_C^v)^{**}(\nabla p_C^*) + (\mathbf{B}_C^v)^{**}, \quad (\text{B.50})$$

where $\mathbf{H}^{**}$, $(\mathbf{D}_C^v)^{**}$, and $(\mathbf{B}_C^v)^{**}$ are the updated momentum coefficients;

2. Interpolate $\mathbf{v}_f^{***}$ using the Rhie-Chow interpolation and compute the new mass flow rate:

$$\dot{m}_f^{***} = \rho_f(\mathbf{v}_f^{***} \cdot \mathbf{s}_f). \quad (\text{B.51})$$

3. Similarly to the fourth step of the SIMPLE algorithm, discretize the continuity equation using the new mass flow rate $\dot{m}_f^{***}$ for one control volume V_C :

$$a_C^{p''} p_C'' + \sum_{F \sim \text{NB}(C)} a_F^{p''} p_F'' = b_C^{p''}. \quad (\text{B.52})$$

Assembling the last equation for the whole mesh and solving it for p'' leads to a new pressure correction field, which in turn is used to correct the velocity field as follows:

$$\mathbf{v}_C'' = -(\mathbf{D}_C^v)^{**} \nabla p_C''. \quad (\text{B.53})$$

4. Correct the mass flow rate, velocity and pressure fields as follows:

$$\begin{aligned} \mathbf{v}_C^{****} &= \mathbf{v}_C^{***} + \mathbf{v}_C'', \\ \dot{m}_f^{****} &= \dot{m}_f^{***} + \dot{m}_f'', \text{ and} \\ p_C^{**} &= p_C^* + p_C''. \end{aligned} \quad (\text{B.54})$$

5. If the number of desired corrections is achieved, set $\dot{m}_f^n = \dot{m}_f^{****}$, $\mathbf{v}^n = \mathbf{v}^{****}$, and $p^n = p^{**}$ and go to step 7 of the SIMPLE algorithm; otherwise, set $\dot{m}_f^{**} = \dot{m}_f^{****}$, $\mathbf{v}^{**} = \mathbf{v}^{****}$, and $p^* = p^{**}$ and return to step 1 of the PISO correction loop.

In the original proposal, Issa, Gosman, and Watkins [56] advocate that iterating twice over the pressure equation is enough to obtain an accurate solution.

C – RESIDUALS IN OPENFOAM

In CFD, the discretization procedure yields a linearized system of algebraic equations that are solved by an iterative method. The iterative process has to be stopped at some point. To evaluate when to stop, many techniques have been proposed [41–43], most of them based on the residual value computed after each iteration. For example, take a linear system of the form

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad (\text{C.1})$$

where $\mathbf{A} \in \mathbb{R}^{N \times N}$, $\mathbf{x} \in \mathbb{R}^N$ is the solution vector, and $\mathbf{b} \in \mathbb{R}^N$. Using an iterative method to solve this system, we can calculate its residual after each iteration by

$$\mathbf{r}^m = \mathbf{b} - \mathbf{A}\mathbf{x}^m, \quad (\text{C.2})$$

where the superscript m represents the current iteration count and $\mathbf{r}^m \in \mathbb{R}^N$.

In order to avoid false convergence, most solvers calculate a normalized version of $\mathbf{r}^m$. Moreover, since $\mathbf{r}^m$ depends on the value of $\mathbf{x}^m$, it is a good practice to scale $\mathbf{r}^m$ to take out the magnitude of $\mathbf{x}^m$. Therefore, OpenFOAM uses a L1-norm to normalize $\mathbf{r}^m$ and the following procedure to obtain the scaling factor:

1. set the reference value as the average value of $\mathbf{x}^m$, as follows:

$$x_{ref} = \frac{\sum_{i=1}^N x_i^m}{N}, \quad (\text{C.3})$$

where x_i^m is the i^{th} component of $\mathbf{x}^m$;

2. define the following vectors:

$$\mathbf{w}_A = \mathbf{A}\mathbf{x}^m; \quad (\text{C.4})$$

$$\mathbf{p}_A = \mathbf{A}\mathbf{x}_{ref}, \quad (\text{C.5})$$

where $\mathbf{x}_{ref} \in \mathbb{R}^N$ with all components equal to x_{ref} ;

3. calculate the scaling factor as

$$F_s = \|(\mathbf{w}_A - \mathbf{p}_A) + (\mathbf{b} - \mathbf{p}_A)\|_1 = \sum_{i=1}^N \left[|(w_A)_i - (p_A)_i| + |b_i - (p_A)_i| \right]. \quad (\text{C.6})$$

Finally, combining the L1-norm and the scale factor of Equation C.6, we obtain the scaled normalized residual, R_s^m , defined as

$$R_s^m = \frac{\|\mathbf{r}\|}{F_s} = \frac{\sum_{i=1}^N |b_i - A_{ij}x_j|}{\sum_{i=1}^N [|(w_A)_i - (p_A)_i| + |b_i - (p_A)_i|]}. \quad (\text{C.7})$$

Note that while the iterative process evolves, the numerator in Equation C.7 goes to zero, whereas the denominator reduces to a constant value. OpenFOAM uses this form of scaled normalized residual to solve the systems of equations for velocity and pressure fields.