A Spectral Element Method for Fluid-Structure Interaction:
New Algorithm and Applications to Intracranial Aneurysms

by

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Thesis
Submitted in partial fulfillment of the requirements for
the Degree of Doctor of Philosophy
in the Division of Applied Mathematics at Brown University

May 2010

The first part of the thesis presents the surface representation of blood vessel walls extracted from medical images, sensitivity to the inlet/outlet boundary conditions, and a hp-refinement study. Our study shows that flow instability in supraclinoid aneurysms is not affected by flow division at downstream branches. However, inlet boundary condition is recommended to be specified upstream of the cavernous segment. The hp-refinement study shows that our spectral element code captures velocity and wall shear stress (WSS) fluctuations.

The second part describes the development and implementation of new fluid solvers with better stability properties than the standard NEKTAR. Due to the strict CFL condition in semi-implicit scheme, the standard NEKTAR over-resolves solutions in time. The semi-implicit scheme is stabilized by sub-iterations with relaxation at each time step. The stability and accuracy of the scheme has been tested with analytic steady solutions, unsteady flows past a cylinder, and pulsatile flows in straight/bend pipes. We also develop a high-order spectral/hp element method for fluid-structure interaction which couples solvers in a partitioned way. Fictitious mass and damping terms introduced to the elastodynamics equation are shown to enhance the stability and reduce the number of sub-iterations. A new boundary condition with spring supports is proposed and its effect on the displacement and stability is investigated.

In the last part of the thesis, we report on flow instabilities and WSS distributions in funnel-shaped bifurcations and aneurysms. Our simulations also show that pulsatile flows in aneurysms are subject to a hydrodynamic instability during the decelerating systolic phase, resulting in high-frequency oscillations in the range of 20-50 Hz. When the aneurysmal flow becomes unstable, both the magnitude and the directions of WSS vectors fluctuate at the aforementioned high frequencies. Impingement regions coincide with the locations of the rupture of infundibulae or progression to aneurysms.
This dissertation by Hyoungsu Baek is accepted in its present form by the Division of Applied Mathematics as satisfying the dissertation requirement for the degree of Doctor of Philosophy.

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Articles in peer-reviewed journals

1. Tomer Anor, Leopold Grinberg, Hyoungsu Baek, Joseph R. Madsen, Mahesh V. Jayaraman, and George Em Karniadakis, *Modeling of large blood vessels*, Wiley Interdisciplinary Reviews Systems Biology, accepted for publication

2. Hyoungsu Baek, Mahesh V. Jayaraman, Peter D. Richardson, and George Em Karniadakis, Flow instability and WSS variation in intracranial aneurysms, Journal of Royal Society Interface, accepted for publication

3. T.S. Jang, Hyoungsu Baek, S.L. Han, and T. Kinoshita, *Indirect measurement of the impulsive load to a nonlinear system from dynamic responses: inverse problem formulation*, Mechanical Systems and Signal Processing, accepted for publication

4. Hyoungsu Baek, Mahesh V. Jayaraman, and George Em Karniadakis, *Wall shear stress and pressure distribution on aneurysms and infundibulae in the posterior communicating artery bifurcation*, Annals of Biomedical Engineering, accepted for publication


7. T.S. Jang, Hyoungsu Baek, and S.L. Han, *new procedure for nonlinear deflection of an infinite beam resting on a nonlinear elastic foundation*, submitted for publication

Articles in conference proceedings

2. Hyoungsu Baek, Mahesh V. Jayaraman, George Em Karniadakis, Effect of aneurysm formation in the supraclinoid internal carotid artery on downstream flow, 34th Annual Northeast Bioengineering Conference at Brown University, Providence, RI (April 4-6, 2008)


4. Hyoungsu Baek, George Em Karniadakis, Suppressing vortex-induced vibrations via passive means, the 9th International Conference on Flow-Induced Vibration 2008 at Prague, Czech Republic (June 30 - July 3, 2008)


6. Hyoungsu Baek, Mahesh V. Jayaraman, George Em Karniadakis, Distribution of WSS on the internal carotid artery with an aneurysm, 60th Annual Meeting of the APS Division of Fluid Dynamics at Salt Lake City, UT (Nov 16-18, 2007)

7. 35th Annual Northeast Bioengineering Conference, Harvard-MIT Division of Health Sciences & Technology, Cambridge, MA, Temporal variation of wall shear stress on the aneurysms in the supraclinoid internal carotid artery (April 3-5 2009)

8. 13th Annual SDSC Summer Institute, UC San Diego, San Diego, CA, WSS on internal carotid artery aneurysm (July 16-20 2007)
Acknowledgments

Finishing this work, I am greatly indebted to many people who have motivated, helped, supported this work. I would like to thank my research advisor and mentor, Professor George Em Karniadakis, for taking me as his student. He is the one who has taught me what research is and how to do it. His curiosity, insight into problems, and methodology has amazed me all the time. I am also grateful for his motivation, guidance, and correction when I need them. I acknowledge all the travel supports for conferences and meetings which have opened my eyes to research widely.

I would like to express my sincere gratitude to dissertation committee members, Professor Chi-Wang Shu, Professor Peter D. Richardson, and Professor Marco Bittencourt for their serving as readers. I am very thankful to Professor Chi-Wang Shu for considerate mentoring and answers, whenever I approach him and ask questions. Professor Peter D. Richardson has been patient and available for every meeting I have have with him. He is the one who has taught me biophysics from the beginning of this research. I have enjoyed collaboration with Professor Maro Bittencourt and owe him many thanks for his comments, suggestions and ideas during our collaboration.

I extend my deep gratitude to Professor Margaret Cheney and Professor Victor Roytburd for taking me as a trainee. I am very thankful to Dr. Leopold Grinberg for demonstrating excellence in research and best practices in high performance computing. I am also aware of and grateful for his guidance into the details of the spectral element method and NEKTAR. I was fortunate enough to work with Professor Steve Dong for a while.

I want to say ‘Gam-sa-ham-ni-da’ to current crunch members for encouragements and questions that I have received and for laughsters and meals that I have shared with them. I also acknowledge that this work was not possbile without codes and tools which have been developed by many crunch members some of whom I have never met. The list of people I want to thank will not end in one or two pages. Although your name is not mentioned here, I owe you a lot, Manimani Saranhamnida Nummulnage.

Lastly, I would like to acknowledge supports from the NSF. Simulations were performed on high-performance computers at PSC, NICS, NAVY DSRC and ARSC.
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C.1 Eigenmodes of clamped-clamped beam of length 4 mm with an attached spring at $x = 2$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant 0, 1e2, 1e4, and 1e6, respectively.

C.2 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, \text{and } 6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two neighboring springs are set to $0.25 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant 1e2, 1e4, 1e5, and 1e6, respectively.

C.3 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, \text{and } 6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two neighboring springs are set to $0.50 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant 1e2, 1e4, 1e5, and 1e6, respectively.
C.4 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, 6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two adjacent springs are set to $0.75 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5,$ and $1e6$, respectively. 

C.5 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, 6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two neighboring springs are set to $1.0 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5,$ and $1e6$, respectively.

C.6 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.25 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5,$ and $1e6$, respectively.

C.7 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.50 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5,$ and $1e6$, respectively.

C.8 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.75 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5,$ and $1e6$, respectively.
C.9 Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $1.0 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.

C.10 Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.25 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.

C.11 Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.50 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.

C.12 Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.75 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.

C.13 Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $1.0 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.
C.14 Eigenvalues ($\lambda_n$) of (a) clamped-clamped beam of length 4 mm with an attached spring of spring constant $K_s = 0, 1e2, 1e3, 1e4, 1e5, \text{ and } 1e6$ at $x = 2$, (b) clamped-clamped beam of length 8 mm with three attached springs of spring constant $K_s = 1e2, 1e4, 1e5, \text{ and } 1e6$ at $x = 2, 4, 6$, (c) clamped-clamped beam of length 8 mm with five attached springs of spring constant $K_s = 1e2, 1e4, 1e5, \text{ and } 1e6$ at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. (d) clamped-clamped beam of length 16 mm with five attached springs of spring constant $K_s = 1e2, 1e4, 1e5, \text{ and } 1e6$ at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. Right plots are zoom-in of the left plots.
Chapter 1

Introduction: Computer Simulations of Aneurysmal Flow

1.1 Background

An aneurysm is a swelling on blood vessel walls. It is speculated that around 16.6% of people over the age of 30 years harbor an unruptured aneurysm smaller than 1 cm [144]. Among aneurysms in the various parts of the arterial system, the intracranial aneurysm is the most serious because of high mortality rate of 50% and another 50% long term disability in case of rupture. Aneurysms are common in bifurcation areas such as the internal carotid artery (ICA) bifurcation, the root of the posterior communicating artery (PCoA), and the middle cerebral artery (MCA) bifurcation. The most common (46%) location of an intracranial aneurysm is the ICA. Hence, this study focuses on aneurysms on the ICA, more specifically at the root of PCoA and along the supracloniod ICA segment.

Intracranial aneurysms are asymptomatic. Hence, they are found by chance and treatments are recommended because of the risk of ruptures. Not many cases are monitored and even monitoring the growth of an aneurysm involves risks of subject’s exposure to contrast agents or radiation. Measuring and obtaining useful information such as pressure, flow rate, and flow impingement inside aneurysms are hindered by the inconvenience of access to intracranial networks. Wall shear stress (WSS), wall thickness, and wall mechanical properties are beyond the current measurement techniques. Hence, computational fluid dynamics (CFD) simulations along with experiments have been used, because simulations...
are able to deliver much more detailed information of flow which are not available through measurements.

Since the interaction of endothelial cells with hemodynamic forces has been observed \[17, 93\], image-based CFD simulations have been used to obtain the distribution of WSS, and then correlate WSS, pressure and other indicators with the formation and growth of an aneurysm \[21, 138, 24, 68\]. Aneurysmal flow simulations combined with clinical observations show that flow impingement regions inside aneurysms tend to have a particular pattern of WSS/pressure distribution which can be associated with the rupture of aneurysms.

The initiation or growth of aneurysm is not fully understood due to lack of data and difficulty of monitoring in-vivo aneurysms. Although there is no ‘mechanotransduction’ model which explains the initiation of aneurysms on blood vessel walls in response to blood flow \[84\], growth of aneurysms has been modeled and simulated \[48, 24, 81\]. Many studies hypothesize that aneurysms are initiated by mechanical stimuli from blood flow based on in-vitro endothelial cell studies including \[93\]. More specifically, impinging zones and areas of high WSS are conjectured to place an area within a blood vessel wall at higher risk for aneurysm formation. Within an aneurysm, the same factors are correlated to growth in size or rupture. A recent in-vivo animal study \[98\] showed that destructive remodeling involving loss of smooth muscle cells occurs at the region of high WSS and WSS gradient where the flow accelerates. Also, a more sensitive response of endothelial cells to turbulent oscillatory shear rather than to laminar and steady shear has been demonstrated experimentally \[93, 100, 98\]. Hence, this study focuses on computer simulations of unstable flow inside aneurysms and numerical methods which takes wall compliance into account. There are mathematical modeling issues as well as computational challenges.

**Mathematical modeling and computational issues**

- Blood is not Newtonian fluid but a suspension of blood cells and platelets in plasma placing another difficulty in simulations. Various cells in the blood generates non-Newtonian characteristics, because the plasma itself exhibits Newtonian behavior. When the blood moves, these particles interact with plasma and among themselves. Hence, whole blood viscosity are strongly dependent on plasma viscosity, volume fraction of cells, deformability of red blood cells, and aggregation of cells. Hematocrit and red blood cell (RBC) aggregations is known to contribute to shear-thinning and
yield stress properties. However, when the shear rates are sufficiently high ($\geq 100s^{-1}$), blood is treated as a Newtonian fluid, which seems to be a reasonable assumption in large arterial flow simulations [90].

- Cerebral arteries are composed of three distinct sub-layers: intima, media, and adventia. The thickness and mechanical strength of the intimal layer are insignificant and may be neglected mechanically. The medial layer contains smooth muscle cells which contract and relax to change the vascular diameter. The adventia and medial layers have collagen and elastin fibers which bear the pressure load along with Glycosaminoglycans (GAGs). Elastin can withstand over 300% strain and return to its undeformed state. Collagen adds stiffness and strength to the artery material matrix.

- Small region of interest in the arterial network is investigated due to limited computational resources and expensive computational cost, and upstream/downstream vessels are truncated near the region of interest. Patient-specific simulations require patient-specific boundary conditions which are not available in most cases. Hence, inlet/outlet boundary conditions are modeled mathematically. However, huge variations of topology of networks and flow conditions among subjects require accurate measurements and ways of imposing boundary conditions which make solution less sensitive to boundary conditions. Stochastic and multiscale nature of downstream network requires advanced and computationally light outlet boundary conditions for velocity and pressure.

- Material and geometric nonlinearity is a challenging problem in solid mechanics, because such nonlinearity lead to expensive Newton-Raphson type iterations. The blood vessel is almost incompressible, and low order methods suffer shear locking. Moreover the thin wall structure may cause geometric locking. However, high-order spectral methods is known to overcome such problems [64].

- The peripheral boundary is usually assumed to have constant pressure in most simulations, which is not reasonable. For example, part of the ICA is embedded in tissues or part of it goes through base skull bones. Near the anterior cerebral artery (ACA)/MCA bifurcations it is immersed in the cerebrospinal fluid (CSF) which is under pulsating motion [8]. To model the peripheral environment is an essential step of blood
flow simulation in compliant vessels. This will also enhance the stability and reduce the computational cost thanks to the effective increase of density and stiffness of blood vessel walls. Obtaining wall thickness and properties is another technical challenge in arterial flow simulations.

- The nonlinear convective term in the Navier-Stokes equations and incompressibility are posing challenges. When the nonlinear term is treated explicitly, the time steps are severely restricted in the spectral method. When compliance of boundary is considered, nonlinearity in the equation gets even stronger, because the location of interface is not known a priori and boundary movements depend on the pressure distribution in the fluid, creating a strong nonlinear problem.

- Simulations of blood flow in compliant vessel walls suffer numerical stability issues even for a short segment of blood vessel, when the density of blood vessel is close to that of the blood and the structural stiffness is small.

Most aforementioned blood flow simulations in brain aneurysms are performed with fluid solvers based on the linear finite element method. However, we demonstrate that aneurysmal flows tend to become unstable due to shear layer instability and resolving flow instability requires high-order spatial and temporal accuracy. Moreover, due to prohibitively expensive computational costs, walls are assumed to be rigid in general and compliance is ignored along with many simplifications. Hence, in this study, we try to tackle challenges in simulation of unstable aneurysmal flows in compliant aneurysms. We focuses on the implementation of high-order spectral element method for stable strongly-coupled fluid-structure interaction (FSI) with unstable aneurysmal flow in mind.

**Fluid-Structure Interaction**

Main difficulties in bioflow fluid-structure interaction are moving boundaries, stability, and strong nonlinearity in both fluid and solid subdomains. To address moving boundary problems in bioflow, Peskin developed immersed boundary method for the motion of heart valves which works well when moving parts are fully embedded in fluid [111]. This is one of meshless methods in which meshes boundaries are not conforming the solid boundaries. For blood flow simulations in compliant vessels, Figueroa et al. developed a coupled momentum method which include the vessel wall deformation as a fluid boundary condition.
through weak formulations [44]. However, it is more general to model blood flow and vessel wall motions by the incompressible Navier-Stokes equations and 3D elastodynamics equations, respectively. In solving such equations, there are two approaches, i.e. monolithic and partitioned. A monolithic solver solves flow and structure in a single code [11, 62], while partitioned one uses separate codes for different domains [43]. Partitioned solvers with sub-iterations have been used because of modularity which makes maintenance and upgrade of each solvers easier. Although a partitioned approach can suffer numerical instability, it is more advantageous in adopting efficient fluid or solid solvers available than monolithic approach.

In more general fluid-structure interaction problems such as particulate flows or free surface flows, remeshing can be computationally challenging. The arbitrary Lagrangian/Eulerian finite element formulation was developed by Hughes et al. [69]. Glowinski et al. proposed fictitious domain formulation, which constrains the fluid motion inside and on the particle boundary using Lagrange multipliers particularly for particulate flows [54, 53]. Tezduyar et al. developed deforming spatial domain/stabilized spacetime method [133].

1.2 Thesis outline

In this thesis, we aim to implement stable strongly-coupled fluid-structure interaction scheme based on the high-order spectral element method: each solvers are parallel, scalable, and efficient; code is modular and upgrading each solvers should be straightforward; code is stable at small density ratio and stiffness. Moreover, we develop and implement a sub-iteration scheme and a fully-implicit scheme whose time steps are not restricted by CFL conditions; such schemes can make expensive FSI simulations more practical. We also propose boundary conditions which models tissues, bones, and tethers which surround blood vessels walls. Very interesting flow instability in the intracranial arterial network, more specifically in aneurysms are observed. Main contributions of this thesis include

- implementation of smooth surface reconstruction from straight faces of polygonal meshes (chapter 2)
- development of sub-iteration scheme of semi-implicit discretization of advection-diffusion equations (chapter 4)
• analysis of stability of sub-iteration scheme (chapter 4)

• analysis of effect of relaxation on stability and range of relaxation parameter for stable relaxation (chapter 5)

• introduction of fictitious damping for the stabilization of fluid-structure interaction (chapter 5)

• analysis of effect of fictitious mass and damping on stability (chapter 5)

• modeling peripheral environments with spring-supported elements (chapter 5)

• finding flow instability in aneurysms and in the circle of Willis (chapter 6)

This thesis is composed of 7 chapters and each chapters are summarized as follows:

• Chapter 2 describes a procedure to create surface meshes from patient-specific medical data. Three bottle-necks are addressed: segmentation with manual editing, surface discretization, and isoparametric smooth surface reconstruction. Solutions are proposed for each problems.

• Chapter 3 explains sensitivity test performed to measure the effect of inlet geometry and outlet pressure on the wall shear stress and possible instability. A hp-refinement test is performed to prove that flow instability is not due to a numerical artifact.

• Chapter 4 reports development and implementation of sub-iteration scheme and fully-implicit scheme which are stable at large time step $\Delta t$. Stability and accuracy tests are performed. Eigenvalue analysis of sub-iteration scheme is carried out to show superior stability.

• Chapter 5 describes solid solver, StressNEKTAR, and coupling with the fluid solver, NEKTAR presented in chapter 4. Accuracy of the solid solver is tested. Fictitious mass and damping are proposed and their stabilizing effects are analyzed. Numerical simulations prove that they enhance stability and save the computational cost. Moreover, new boundary conditions which mimics the peripheral environment are implemented and their effects on deformation, stress field, and stability are studied.

• Chapters 6 and 7 delineate unstable blood flows and WSS/pressure distribution in patient-specific geometries published in [6] and [5], respectively. More specifically,
aneurysmal flows inside wide-necked aneurysms tend to become unstable resulting in velocity fluctuations in the aneurysm sac and WSS fluctuations on the wall. Most simulations are done with rigid wall models. A FSI simulation shows that compliance of wall may attenuate or amplify such flow instability depending on the material stiffness.
Chapter 2

Image-based Simulations : from Medical Images to Computational Meshes

It is not surprising that geometric models for simulations of aneurysmal flows have shifted from simple idealized geometries to patient-specific geometries due to the importance of geometric sensitivity [21, 140]. Hence, blood flow simulations require computational meshes from medical images. Medical imaging technology has been advanced in a very rapid pace, but obtaining computational meshes of a good quality is a challenge. For example, intracranial arteries range from 5 mm to submillimeter in diameter. Such diameter changes along the vessels pose great difficulties in segmentation process. Bone structures close to vessels, two adjacent vessels, and thin blood vessel walls prevent the process from being automated. Visualization through image segmentation of organs in medical images has been under active research. Creating quality meshes from medical images are even more challenging and it is an active research topic itself. The process from medical images to computational meshes is well explained in [20] and summarized here.

1. anonymize medical images and export

2. remove noises and resampling, if necessary, for isoresolution images

3. locate the boundary of blood vessels using intensity level (threshold method) as an initial guess
4. refine the location using more advanced models such as deformable walls
5. remove small branches and/or fill in holes
6. truncate inlet/outlet vessels and make extensions for boundary conditions
7. discretize surface
8. discretize volume

Medical image modalities used in this study are computer tomography angiography (CTA), digital subtraction angiography (DSA), and magnetic resonance angiography (MRA). The image quality varies depending on the image modality. Hence, I briefly describe the medical image sources and then image segmentation methods. Three bottle-necks are addressed and solutions are proposed: defining the blood vessel walls from images, surface discretization, and isoparametric representation of anatomically-correct blood vessel walls in high-order method. I propose a combination of available software tools as a fast and robust pipe-line that have been established and shown for an intracranial network with more than 200 branches. At the end of this chapter, a method of geometry modification which is used in our hypothetical studies is presented.

2.1 Image modality

Image data provided in the DICOM format are obtained from CTA, three-dimensional DSA, or MRA. These image data are anonymized to remove any patient specific data. The resolutions and noise levels of the dataset are widely spread, i.e. the resolution ranges from 0.1 mm to 0.5 mm per pixel. Among the noninvasive imaging modalities, CTA is the most widely used in various clinical applications including cardiac, head and neck, and abdomen with a spacial resolution of under 0.5mm in all three dimensions. Imaging brain aneurysms and blood vessels with CTA can not avoid bright bone structures which make the segmentation and visualization much more difficult because image intensity of bone structures are in the same range of lumen. MRA is another non-invasive imaging technique for blood vessels. The spatial resolution of MRA is not as good as CTA. DSA is a technique to visualize blood vessels by subtracting a non-contrast image from a contrast image. This suppresses the surrounding bones and tissues significantly and the resulting image is much
better than CTA or MRA. However, DSA doubles the radiation dose for CT imaging and also requires perfect alignment of the two sets of images. DSA works better in brain imaging than lung or heart imaging because the motion of vessels in the brain is not as large as those on the lung or heart. Hence DSA is widely used in head and neck imaging where motion is minimal. Although advances in medical imaging have improved the quality significantly, images are easily degraded by noises and artifacts such as blurring and aliasing.

2.2 Finding blood vessel walls - Amira

Segmentation is a typical classification process which maps each volume element or voxel into groups. The only available information in the images is intensity in grey-scale. Usually this is not enough, and researches try to exploit known anatomical information. Image segmentations and visualizations are useful for many different applications, for example, diagnosis, study of anatomical structure, treatment planning, and computer-integrated surgery. Recently, image-based simulations of blood flow, joint contact, and hand movements have revealed tremendous new information and better ideas about biophysics phenomena which are not available otherwise. Moreover image analysis for area, volume, or relative position changes are need in comparative studies among normal and controlled subjects.

Detection and segmentation of arteries are challenging because of size variations from cm to submillimeter in diameter as well as poor image qualities. The intracranial blood vessels are passing through bone structures, and image intensity of bone structures are close to that of blood vessel resulting in great difficulties in differentiating them. As mentioned above, DSA technique can be applied to imaging neck and head.

Classical segmentation

Among the available segmentation methods, threshold is simple and can be effective when the image quality is good and if the bone structures are removed. It has been commonly used in image segmentation to obtain initial locations for more advanced segmentation methods. However, this method is very sensitive to noises and intensity changes which may come from changes in the contrast agent density.
Deformable models with Levelset representation

Since the introduction of deformable model by Kass et al. [79], parametric and geometric deformable models are actively used in image segmentation. The success of these methods are ascribed to the representation of surfaces as a level set of higher dimensional function and the development of numerical method for Hamilton-Jacobi equations describing the curve (surface) evolution. This can handle any topological changes of the geometry, e.g. splitting, merging of blood vessels. Even more advanced methods are under development and give satisfactory results for visualization purposes. However, automatic computational mesh generation is not available yet. Such methods are implemented in commercial/free toolkits. For example, Amira (Visage Imaging, Richmond Australia), MT (http://www.vmtk.org), Slicer (http://www.slicer.org), and itk-SNAP (http://www.itksnap.org) have been used for visualization purposes. Segmentations with deformable model were tested with available patient-specific images. The most serious obstacle is leaking of deformable surfaces into neighboring bones and adjacent arteries or veins. When the image resolution is coarser than the thickness of the blood vessel walls, boundaries (sharp changes in intensity) between two vessels or between a vessel and neighboring bones are smeared and the deformable walls do not stop there, resulting in leaks. Another problem of deformable model is that the deformable surface can not proceed into small vessels due to the diffusion term which is introduced to remove wrinkles on the deformable wall. Inside small vessels, the front surface of deformable walls have high curvatures, which make the diffusivity term dominant in the evolution equation and deter the expansion of the deformable walls.

Unavoidable manual editing

Among these tools, Amira seems to work well with medical images that we have. The manual editing feature and graphical user interface allow inexperienced users to perform segmentations. Smoothing and threshold-based segmentation give blood vessel surfaces of reasonable quality. However, due to the image artifacts, small arteries, and empty holes, generating surface meshes from segmented images can not be automated. Extracted vessel walls need smoothing, filling-in, and truncation. Hence, Amira has been tested, and manual editing of surfaces and volume proves to be convenient and does not need experienced operators thanks to a graphical user interface.
2.3 Surface discretization - VMTK + Gridgen

Amira can produce water-tight smooth surfaces after manual editing and surface extraction. However, discretizing anatomical curved and tortuous surfaces using a mesh generator, Gridgen, is not satisfactory. Hence, extra lines had to be drawn to discretize the surfaces, which was time-consuming. Hence, VMTK tool to split arterial network into branches has been tested, and discretizing split branches proves to be very robust and to save time in the mesh generation process. This new method is tested in a large geometry shown in Figure 2.1 and split branches are shown on the right of Figure 2.1; for details of VMTK commands please refer to Appendix A. Moreover, it is less sensitive to the level of operator skill. After generating water-tight surface models, volumetric meshes are generated from those surface models.

Figure 2.1: Entire geometry of intracranial arterial network of an aneurysm patient (left) and split branches using VMTK (right). Colors on the right represent different pieces of branch which can be easily discretized using Gridgen. The meshes on the right is not the computational mesh but only for viewing clarity.
2.4 Isoparametric reconstruction of smooth curved surfaces using SPHERIGON

Gridgen generates linear finite elements and all face elements have straight faces. Since p-refinement is more efficient than h-refinement, simulations based on the spectral/hp element method prefer large elements and solutions are resolved through p-refinements. Due to the high curvatures and complicated topology of patient-specific geometries, especially near the aneurysms in the ICA and cavernous ICA segment, small elements are used. Moreover, when the wall shear stress (WSS) is one of the main interest in aneurysmal flow simulations, discontinuity in the normal vectors along the sharp edges or vertexes may significantly degrade the quality of distribution of WSS. Hence, first to increase the size of elements and make smooth surfaces, boundary faces of linear finite elements have to be projected into curved surfaces interpolating vertexes on the surface. In our code NEKTAR, a visualization algorithm, SPHERIGON, is implemented to construct smooth $C^0$ surfaces. The faces of tetrahedral elements at the vessel walls are projected onto curved surfaces generated by SPHERIGON which requires the position of the vertexes and the corresponding normal vectors. For details of the algorithm, we refer the reader to [92].

Convergence test with known normal vectors at the vertexes

When a surface is reconstructed with SPHERIGON algorithm, the geometry and solution should converge to a certain limit. In order to confirm this, steady flow is simulated in a straight pipe, because a geometry of straight pipe can be described algebraically and used as a reference. This study shows that both geometry and solution converges as the polynomial order increases. The analytic solution is given as the Womersley flow. A pipe of diameter 1 mm is simulated with flow rate 9.97 ml/min and mean velocity 0.212 m/sec, and the Reynolds number 55.70. From the flow rate $q_s$, the WSS is obtained analytically by $4\mu q_s/\pi R^3$, where $R$ is the radius and $\mu$ is the viscosity of fluid. We calculate $L_{\infty}$ errors in velocity and $L_2$ errors in WSS against analytic solution under steady flow condition. Figure 2.2 shows that visually there is no difference between geometries using SPHERIGON reconstruction and algebraic expression of the cylinder. The velocity field and WSS on the wall also show the spectral convergence for polynomial order $p$ as in Figure 2.3 and 2.4.
2.5 Procedure of “virtual surgery”

For simulations in chapter 7, a geometry needs to be modified for hypothetical studies. For example, if we want to compare flow changes due to aneurysm growth, the aneurysm is digitally removed since the images before the aneurysm develops are not available. Here I explain the details of the manual procedure in mesh generation software, Gridgen. This virtual surgeries are done for simulations of hypothetical cases in chapter 7.

In order to generate smooth surface patches which will replace aneurysm walls, we used editing and surface generation tools in Gridgen. More specifically, we relied on two features of Gridgen: drawing smooth splines and creating smooth surfaces when the boundary lines are defined. These interpolating lines are indicated as pink lines in Fig. 2.5 (a). In order
Figure 2.3: $L_\infty$ error versus polynomial order (p). ‘cyl’ corresponds to velocity errors in a pipe created with algebraic expression. ‘sph’ corresponds to velocity errors in a pipe reconstructed with SPHERIGON algorithm implemented in NEKTAR.

to make the procedure more understandable, we describe the steps taken to create a single smooth surface patch; see the red solid surface in Fig. 2.5 (a). As a first step, the entire aneurysm and parts of parent vessel around the neck of the aneurysm were removed. This was possible because the original patient-specific aneurysm geometries consist of smooth surface patches. When the PCoA comes out of the aneurysm, i.e. the aneurysm in patient C and the upstream aneurysm in patient D of chapter 7, we did not modify most part of the PCoA except the junction with aneurysm, and reused the PCoA to draw the scaffolding lines. Splines were drawn from one side of the ICA to the other side of the ICA or from the ICA to the PCoA, e.g. line G1-G2 and G5-G6, respectively in Fig. 2.5 (a). More splines such as line G3-G4 were drawn to define the boundary lines of a patch. Using these splines, Gridgen generates rectangular-shaped patches. Finally, on top of these patches, surface discretizations were created, followed by volumetric discretizations. The completed aneurysm-removed models of patient C and D are compared with the original aneurysm geometry in Fig. 2.5 (b-1, b-2, c-1, c-2).
Figure 2.4: WSS errors in pipe flows versus polynomial order (p). ‘Cylinder’ corresponds to WSS errors in a pipe created with algebraic expression. ‘Spherigon’ corresponds to WSS errors in a pipe reconstructed with SPHERIGON algorithm implemented in NEKTAR.

2.6 Conclusions

In this chapter, three practical bottle-necks in mesh generation procedure are addressed: segmentation with manual editing, surface discretization, and isoparametric representation of surfaces. Surface extraction and manual editing with Amira has been used successfully for several patient-specific meshes. Procedures of branch splitting and extrusion using VMTK have been tested and proved to be efficient through a case of a large arterial network composed of more than 200 arteries. Reconstruction of smooth surfaces with SPHERIGON algorithm and projection of spectral element faces are proposed and implemented in NEKTAR. Such surface reconstruction has been used in many large scale simulations in [57] as well as in this thesis. Geometry modification using Gridgen for hypothetical studies is also explained which has been used for simulations in chapter 7.
Figure 2.5: Example of making a smooth surface patch using the Gridgen mesh generator, and comparison between original aneurysm models and the generated aneurysm-free models. (a) The pink grid represents the geometry of the aneurysm and the red shaded surface represents a smooth surface patch generated using red dotted lines as scaffolding (boundary lines). The line G1-G2 starts from one side of the ICA wall and connects to the other side of the ICA wall. The line G3-G4 is on the ICA wall. The line G5-G6 is drawn from the ICA wall to the PCoA wall. Gridgen generates the red smooth surface from the given four boundary lines. (b-1, b-2) Two views of the overlap of the aneurysm model (CA) and aneurysm-removed geometry (CI) of patient C in chapter 7. (c-1, c-2) Two views of the overlap of the two aneurysm model (DT) and the aneurysm-free model (DI) of patient D. (b-1) and (c-1) show geometry viewed from the direction indicated with arrows in (b-2) and (c-2). (b-2) and (c-2) are views from the bottom of the aneurysms.
Chapter 3

Sensitivity Study

3.1 Introduction

Sensitivity studies are done routinely in numerical simulations to understand how much solutions are dependent on parameters or any specific simulation condition. In this chapter, three kinds of sensitivity study in image-based patient-specific simulations are performed.

- Patient-specific blood vessels are not simple rectangular or straight tubular geometries. Hence, it is not obvious where to truncate inlet/outlet vessels. Even though CFD simulations can give an accurate picture of aneurysmal flow as shown in validations with an in vitro experiment [1], this accuracy is possible only when the correct and plausible boundary condition is given near the aneurysm. Obtaining accurate, patient-specific 3D velocity boundary conditions, however, is neither practical nor possible in most cases of simulations. Hence, simplified velocity profiles are imposed at the inlet. It is, therefore, important to investigate the effect of the inlet vessel geometry, namely sensitivity of the numerical solution to the inlet boundary conditions.

- In simulations of flow on the arterial networks with multiple outlets, pressure boundary conditions at the outlets may change flow division at branches, which results in huge differences in flow rates downstream and WSS distribution. In such cases, constant pressure condition should be avoided because flow division is solely determined by the resistance of the downstream vessel segment in the computational domain. However, constant pressure has been used for the pressure boundary condition at the outlets, since the pressure measurement at the outlet vessels or the relation between the flow
rate and pressure are not available in most cases. Hence, we will confirm that different
types of pressure boundary condition and changes in flow division do not affect flow
characteristics in the regions of interest. More specifically, sensitivity of flow instability
and WSS distribution at the supraclinoid segment is investigated when the flow rate
changes at the ICA bifurcation into MCA and ACA substantially.

- Blood flows are subject to instability, as we will present in Chapter 6 and 7. However,
it is a legitimate question whether instability and velocity fluctuations are numerical
artifacts or physical phenomena. A hp-refinement study is carried out and presented
to make sure that our spectral element code with a moderate polynomial order can
accurately capture velocity fluctuations of 30-50 times cardiac fundamental frequency.

Four subjects are used for sensitivity test in this chapter. Three subjects A, B, and C
in Table 3.1 are used for sensitivity of inlet geometry, and three subjects B, C, and D in
the same table are used for outlet pressure boundary condition. One subject C with two
aneurysms in proximity is used for a hp-refinement test with flow instability.

3.2 Inlet geometry sensitivity

In order to obtain physiologically correct results through CFD simulations, geometric mod-
eling is the most important preprocessing task. It is not surprising that geometric models for
simulations in aneurysms have shifted from simple idealized geometries to patient-specific
geometries due to the importance of geometric sensitivity [21, 140]. Moyale et al. [101]
investigated the effect of the inlet condition on WSS and oscillatory shear index (OSI) in
the common carotid artery (CCA) bifurcation by generating secondary flow with extended
straight pipe or helical pipes with varying curvatures. They claimed that WSS on the bifur-
cation is not sensitive to inlet flows generated with long helical pipes, and hence the velocity
profile obtained at the end of such pipes may be used as a boundary condition for general
purposes. They attempted to “synthesize” a proper inlet condition and hence use small
computational domains in their simulations. However, since aneurysms in the supraclinoid
ICA have much more complicated and tortuous upstream vessels than the helical pipe, the
flow generated from the helical pipe may be far from realistic. The sensitivity study of
Castro et al. [18] implied that the aneurysm should be considered as part of a circulatory
system and not a standalone system with idealized input and output. They investigated
the influence of the parent artery geometry and concluded that the computational domain should contain quite a long upstream parent vessel. In particular, they compared two extreme cases of parent vessel geometry. One model was truncated 1cm upstream from the aneurysm, and then extended with a straight pipe. The other had quite a long original parent vessel geometry. Unfortunately, their results did not suggest how far upstream the domains should be extended for CFD simulations, or how sensitive WSS is to a change in the upstream parent vessel.

Motivated by the aforementioned results, we used a long parent vessel in our study to create a more accurate inlet flow and to understand the development of realistic secondary flow before reaching the aneurysm. Moreover, in the present study we aim to understand the sensitivity of WSS distribution to the inlet boundary condition, a critical step for future accurate simulations of aneurysms. In this chapter, we report a series of highly-resolved parallel spectral/hp element simulations with patient-specific 3D models and quantify the sensitivity of WSS on the geometry of parent vessels through qualitative and quantitative comparisons of WSS distribution and WSS averaged over small patches on the aneurysms.

For comparison purposes, ten geometric models were generated from the three vascular systems. For each aneurysm, the first variation was a shorter inlet vessel with only one bend, the cavernous ICA segment. The second variation was a longer inlet vessel that includes one more bend of the ICA, the lacerum ICA segment. The third variation was generated by including three bends upstream from the aneurysm and the inlet end was chosen in the relatively straight distal cervical segment as clearly shown in Figure 3.1. Hence, qualitatively

Table 3.1: Dataset for 3D patient-specific models. The units of image size and resolution are pixel and $10^{-1} mm/pixel$ respectively.

<table>
<thead>
<tr>
<th>Patient</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>W-necked</td>
<td>N-necked</td>
<td>Two n-necked</td>
<td>Inf.</td>
<td></td>
</tr>
<tr>
<td>Parent</td>
<td>ICA</td>
<td>ICA/PCoA</td>
<td>ICA/PCoA</td>
<td>ICA</td>
<td></td>
</tr>
<tr>
<td>Turn</td>
<td>sharp</td>
<td>smooth</td>
<td>tortuous</td>
<td>tortuous</td>
<td></td>
</tr>
<tr>
<td>Size</td>
<td>8x8x10</td>
<td>6x6x3</td>
<td>3x4x2.5, 4x4x3</td>
<td></td>
<td>mm</td>
</tr>
<tr>
<td>Image Size</td>
<td>512x512x312</td>
<td>512x512x396</td>
<td>512x512x470</td>
<td>512x512x518</td>
<td>pixs</td>
</tr>
<tr>
<td>Resolution</td>
<td>4.88x4.88x6.25</td>
<td>3.38x3.38x3.38</td>
<td>3.73x3.73x6.25</td>
<td>4.88x4.88x6.25</td>
<td>$10^{-1} mm/pix$</td>
</tr>
<tr>
<td>Data Source</td>
<td>CT</td>
<td>3D-Digital Sub.</td>
<td>CT</td>
<td>CT</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Angiography</td>
<td>Angiography</td>
<td>Angiography</td>
<td>Angiography</td>
<td></td>
</tr>
</tbody>
</table>
speaking, the length of the each parent vessel varied from short to intermediate and long. We compare WSS distribution in two different scales: spatially averaged wall shear stress (SAWSS) on small patches of radius 1-1.5 mm (S1) and SAWSS on larges patches of radius 3-4 mm (S2). Comparison in all two scales shows similar trends qualitatively. Small patches turn out to be very useful, because SAWSS on small patches enables us to interpret the WSS difference from the hemodynamics point of view and associate WSS distribution with the flow structure. Hence, most comparisons are made in the scale S1 in the following sections. Small patches consist of faces of curved elements and these patches are identical among variations of specific patient data for fair comparison since discretization in the aneurysm does not change among models as explained above. In the following, we first present details on the geometric models and the simulation parameters, and subsequently we present the results with discussion.

3.2.1 Geometry reconstruction

The dataset of patient A in Table 3.1 was resampled to make it isotropic with the final resolution being $0.488 \times 0.488 \times 0.488 \, mm$ per pixel in the $x$, $y$, and $z$ directions. This dataset was manually extracted using an in-house Matlab tool, which allows users to pick any $x$, $y$, or $z$ slices for the best viewing angle. The boundaries of blood vessels were extracted based on the intensity and the maximum intensity gradient. The extracted vessel walls were smoothed and all smoothed rings were connected to make surfaces representing vessel walls. The dataset of patient B in Table 3.1 is isotropic; it has a higher resolution, and was given as a subtracted data set with bony structures removed. Using pixel intensity, an isosurface represented by polygonal meshes was obtained. The decrease of the ICA diameter is observed in the supraclinoid segment between the ophthalmic and posterior communicating artery bifurcation as pointed out by [56].

For patients A, B, and C data, the surface geometries from Matlab were exported to Gridgen (Pointwise Inc, Fort Worth, TX), a mesh generation software. Using Gridgen, water-tight surface models were generated. For patient A, the inlet vessel was modified to make the turns straighter than they are in the original geometry. After generating water-tight surface models, meshes were generated from those surface models. To maintain the same meshes and same surface shapes in the aneurysms, the entire domains were separated into three, two, and three blocks for patients A, B, and C, respectively. For each patient,
the meshes in the aneurysm part did not change but the inlet meshes are different. As a final step, tetrahedral spectral elements were generated in the lumen and aneurysm.

Most surface faces of boundary elements, except some elements in recessed corners, were curved using a polygonal interpolation algorithm [92]. Even though the numerical solution itself guarantees only $C^0$ continuity, the WSS discontinuity turns out to be mild enough not to need any smoothing. This enabled us to use larger elements with total number of spectral elements $40,000 - 80,000$ for the vessels of length $100 \text{ mm}$. Unstructured meshes with tetrahedral elements were used and the typical length of edge of an element was $0.5 - 0.8 \text{ mm}$, which is two or three times as big as the size of pixel of the source image. Inside each tetrahedron, high-order interpolation is employed as explained in the next section.

3.2.2 Numerical simulation setup

Blood is assumed to be an incompressible Newtonian fluid with kinematic viscosity $3.80 \times 10^{-6} \text{ m}^2/\text{s}$. The blood vessel walls were assumed to be rigid; elasticity may reduce WSS level and hence the rigid vessel wall gives more or less similar and conservative results, as Torii et al. reported [136]. So the fluid motion is governed by the incompressible Navier-Stokes equations with the no-slip boundary condition on the fixed wall. Inlet and outlet boundary conditions are imposed by the Womersley solution and constant pressure condition, respectively.

The incompressible Navier-Stokes equations were solved with parallel NEKTAR [77], which implements the spectral/hp element method. This solver employs a high-order splitting scheme and each time step is composed of three substeps. At the first substep, the solver updates the previous time step solution with the explicit nonlinear convection term. Then, the pressure is obtained by a Poisson equation using the updated intermediate velocity and Neumann pressure boundary conditions. At the third substep, the next time step velocity is obtained by solving three inhomogeneous Helmholtz equations. The unknowns, i.e. velocity and pressure, are expressed as a linear combination of a Jacobi polynomial basis. Each tetrahedral element has 35 basis modes, and $C^0$ continuity is imposed at the boundary of the elements. In order to make sure that the flow is well resolved with the meshes and polynomial basis, $p-$refinement sensitivity tests were carried out under steady flow conditions with average flow rate. Comparing velocity and WSS surface integration
Table 3.2: Simulation parameters for the patient A and C models. Re is based on the diameter of the inlet, mean velocity, and assumed kinematic viscosity. $\omega_n$ is based on the radius ($R$) of the inlet, pulsatile circular frequency ($\omega = 2\pi f$), and kinematic viscosity ($\nu$). ‘L’, ‘I’, and ‘S’ stand for long, intermediate, and short, respectively.

<table>
<thead>
<tr>
<th>Case</th>
<th>AL</th>
<th>AI</th>
<th>AS</th>
<th>AM</th>
<th>CL</th>
<th>CI</th>
<th>CS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Patient</td>
<td>A</td>
<td>A</td>
<td>A</td>
<td>A</td>
<td>C</td>
<td>C</td>
<td>C</td>
</tr>
<tr>
<td>Length</td>
<td>L</td>
<td>I</td>
<td>S</td>
<td>S</td>
<td>L</td>
<td>I</td>
<td>S</td>
</tr>
<tr>
<td>VFR (ml/min)</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>mean U (m/s)</td>
<td>0.252</td>
<td>0.28</td>
<td>0.43</td>
<td>0.43</td>
<td>0.170</td>
<td>0.223</td>
<td>0.170</td>
</tr>
<tr>
<td>Re</td>
<td>271</td>
<td>286</td>
<td>355</td>
<td>355</td>
<td>223</td>
<td>255</td>
<td>253</td>
</tr>
<tr>
<td>$\omega_n = R\sqrt{\frac{\nu}{\nu}}$</td>
<td>3.04</td>
<td>2.89</td>
<td>2.33</td>
<td>2.33</td>
<td>3.46</td>
<td>3.027</td>
<td>3.05</td>
</tr>
<tr>
<td>Elements</td>
<td>75536</td>
<td>62548</td>
<td>45326</td>
<td>50478</td>
<td>124845</td>
<td>102878</td>
<td>87002</td>
</tr>
</tbody>
</table>

between a reference simulation (p=4) and p-refined one (p=6) confirmed that differences were less than 4%, where p denotes the order of the polynomial basis. Therefore, all simulations in this study were performed with the polynomials of order p=4, and discontinuity of WSS across elements was confirmed to be negligible.

At the inlet boundary, the Womersley velocity profile, which is the exact solution of pulsatile flow in a straight rigid pipe for a given flow rate, was imposed at the extended inlet. The volumetric flow rate (VFR) profile is shown in Figure 3.2. This profile was taken from the measurements of [94], and then eight complex Fourier coefficients were used to calculate the Womersley profile during simulations. The average flow rate into the ICA is fixed at 200 ml/min for most of simulations. Only for intermediate and long models of the patient B, the average VFR 300 ml/min is used to examine our hypothesis that higher VFR will cause more deviation of WSS distribution between the models. Also, 80 beats per minute (BPM) are used in all ten simulations for heart periodic pumping. Simulations were performed for 1.5 to 2 cycles, and the data from the last cycle are used for comparison and further analysis.

### 3.2.3 Results

For the same VFR, 200 ml/min, the patient A models respond very sensitively to the inlet length variations while the patient B models are shown to insensitive to the change. However, for the higher Re = 270 $\sim$ 350, both models show similar quantitative and qualitative differences among their inlet length variations. The downstream aneurysm in patient
Table 3.3: Simulation parameters for the patient B models. $Re^*$ is based on the diameter of the inlet, mean velocity, and assumed kinematic viscosity. $\omega_n^*$ is based on the radius ($R$) of the inlet, pulsatile circular frequency ($\omega = 2\pi f$), and kinematic viscosity ($\nu$). ‘L’, ‘I’, and ‘S’ stand for long, intermediate, and short, respectively.

<table>
<thead>
<tr>
<th>Case</th>
<th>BL</th>
<th>BIO</th>
<th>BIM</th>
<th>BS</th>
<th>BLH</th>
<th>BHI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Patient</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>B</td>
</tr>
<tr>
<td>Length</td>
<td>L</td>
<td>I</td>
<td>I</td>
<td>S</td>
<td>L</td>
<td>I</td>
</tr>
<tr>
<td>PCoA Length</td>
<td>S</td>
<td>S</td>
<td>L</td>
<td>S</td>
<td>L</td>
<td>L</td>
</tr>
<tr>
<td>Average VFR (ml/min)</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>mean U (m/s)</td>
<td>0.19066</td>
<td>0.22</td>
<td>0.22</td>
<td>0.2</td>
<td>0.2853</td>
<td>0.33066</td>
</tr>
<tr>
<td>$Re^*$</td>
<td>235</td>
<td>253</td>
<td>253</td>
<td>242</td>
<td>353</td>
<td>381</td>
</tr>
<tr>
<td>$\omega_n^* = R\sqrt{\frac{\omega}{\nu}}$</td>
<td>3.49</td>
<td>3.25</td>
<td>3.25</td>
<td>3.41</td>
<td>3.49</td>
<td>3.25</td>
</tr>
<tr>
<td>Elements</td>
<td>62548</td>
<td>38349</td>
<td>63062</td>
<td>58206</td>
<td>62548</td>
<td>38349</td>
</tr>
<tr>
<td>Time Units/Cycle</td>
<td>143</td>
<td>165</td>
<td>165</td>
<td>150</td>
<td>214</td>
<td>248</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>0.001</td>
<td>0.001</td>
<td>0.002</td>
<td>0.002</td>
<td>0.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

C models show more pronounced difference among models than the upstream aneurysm. Moreover, flow in patient C models become unstable, and velocity and WSS fluctuates.

Patient A: wide-necked aneurysm on parent vessels with sharp turns

Case AS differs from cases AI and AL both qualitatively and quantitatively while cases AL and AI show close similarity. Case AS differs from cases AL and AI by more than 60 % in terms of peak SAWSS over the small patches on the aneurysm. In most patches, the shorter the inlet length is, the larger the SAWSS peaks are. Near the dome tip of the aneurysm, however, the case AL or AI has stronger SAWSS peaks as shown in Fig. 3.3(d) and 3.3(g). We define the temporal variations of the SAWSS over the patches as the ratio of the value at the systolic peak to that at the end of the diastole. Both the average WSS and the temporal variations of the SAWSS over the patches are very high near the impinging zone. It is noteworthy that the aneurysm dome has very low WSS but very high temporal variations. Qualitatively, WSS distributions on the surface are quite different, especially near the entrance of the aneurysm. There is hardly any difference between case AI and AL. Some peak spots in the case AS disappear in cases AL and AI. The size of peak WSS spots and the WSS magnitudes in case AL are smaller than they are in the short model, case AS. Along the upstream ICA vessel, differences are more pronounced. The high WSS spots on the top of the first turn (cavernous ICA segment) of case AS is definitely the effect of the
short distance from the inlet boundary condition. Case AL has a peak spot not on the top but on the side of the cavernous ICA, and its magnitude is smaller than that of case AS because of the fully-developed secondary flow of case AL.

**Patient B: narrow-necked aneurysm on parent vessels with smooth turns**

When we test patient B geometries with lower VFR, 200 \(ml/min\), there exists no difference between long and intermediate models and between intermediate and short models. SAWSS completely agree with each other as well as the \(x, y, z\)-components of SAWSS and velocity fields. We compare the flow structures in the parent vessels with different inlet locations. The Womersley inlet profile quickly disappears within three to four inlet vessel diameters downstream. Moreover, the flow structures in long and intermediate models become very similar in the anterior cavernous ICA. This similarity becomes stronger as the flow approaches the aneurysm and it becomes even harder to tell the difference between two models. When the average VFR increases from 200 \(ml/min\) to 300 \(ml/min\), the SAWSSs on the many patches of case BIH and BLH began to deviate over the entire period as shown in Fig. 3.4. We point out that the shorter model (BIH) has higher SAWSS on the patches ‘inside the aneurysm’ while the long model has ‘on the parent vessel’.

**Patient C: narrow-necked two aneurysms on highly tortuous parent vessel**

Visual inspection of WSS on the aneurysm wall does not differentiate three models with different inlet locations. However, SAWSS on the small patches shows very interesting result, as shown in Figure 3.5, where cases CI and CL agree over the cardiac cycle but case CS deviates almost 100 \% from case CI and CL. Three patches show 60 \(\sim\) 100 \% and all of them are on the down stream aneurysm.

### 3.2.4 Discussion

During systole, impinging zones have high WSS peak close to 40 \(\sim\) 50 \(N/m^2\) and the neck of aneurysms also has relatively high WSS due to the high curvature. Regions of low WSS less than 5 \(N/m^2\) are observed in aneurysms over the cardiac cycle and the flow inside the sacular aneurysm seems to be stagnant during diastole. Both high WSS and low WSS is known to be problematic to the health of the vessel walls. Moreover, previous studies of [122] and [49] hypothesized that they are related to the initiation/rupture, and
growth of aneurysm, respectively. Low WSS regions away from impinging zones can have high temporal variation due to extremely low WSS during diastole and somewhat increased WSS at the systolic peak. Hence, high WSS and low WSS could be problematic not because of their magnitudes but because of their temporal variations.

The flow structures in cases BL and BS are very interesting in that the flow impinges the vessel wall just above the aneurysm and separates into two. One follows the ICA and joins the main flow to the bifurcation. The other enters into the aneurysm and sweeps the wall of aneurysm and then swirls up. The swirling is induced by the shear of the main flow with strong axial component but weak in-plane components, since the aneurysm offsets the parent vessel a little, and the protruding daughter lobule totally breaks the symmetry of the geometry and the flow. When the flow impinges the wall and sweeps the aneurysm, the pressure rises near the impinging point and WSS increases at the neck of the aneurysm. A second impinging point is formed inside the aneurysm when the sweeping flow is blocked near the dome of parent aneurysm. This impinging zone has higher pressure as well and is located near the neck of the daughter, lobule which is removed partially in BL and BIM.

The correlation between high WSS and high pressure is clear. There seem to be three cases of high WSS region: reduced cross sectional areas, sharp turns, and sharp corners such as the neck of a saccular aneurysm. When a vessel wall is in close contact with the high tangential velocity zone of the blood flow, the velocity gradient becomes large, and the pressure decreases at the wall. However, if the flow hits the wall perpendicularly, it stalls at the intersection between the extended line of incoming flow and the wall, and consequently the pressure increases in the stagnation area. Near this high pressure spot, the flow separates radially and then joins the main stream, accelerating and causing high velocity gradient and high shear stress. Hence, high WSS and locally elevated pressure seem to be correlated except for high WSS from the reduced cross-sectional area.

We also found some features which do not follow our intuition. The WSS vectors do not change their direction during the cardiac cycle but their magnitudes do. The WSS peak spots in the normal vessel occur not in the outside tip of turn but at the sides (the binormal vector direction when considering the skeletonized curve of the blood vessel) of turns because of the secondary flow structure. Without this secondary flow, the WSS peak spots are at the outside tips of turns as observed in the cases AS and BS. Hence, the high WSS peaks observed in many experiments and simulations seem to be the effect of
parallelized flow without planar velocity components. The locally elevated pressure peaks exist at the outside tip of turns to balance the centrifugal force.

Surprisingly, the way the fully developed flow passes a L-shaped turn is totally different from that of the Womersley profiles in case AS, which does not fully develop secondary flow structures due to the short and more or less straight inlet as manifested in Fig. 3.7. The arrows in Fig. 3.7(a) clearly show that the turn of the Womersley profile flow is more violent in that it hits hard the wall near the apex of the turn, deflects to the other side, and sweeps the wall making a streak of relatively high WSS along the path of the high velocity core. However, fully developed flows (cases AI and AL) make much more gradual and graceful turn because of the secondary flows. Their gaps between the isosurface and the wall are much larger than those of cases AS and AM. This means that applying the Womersley profile without secondary flow structure at short upstream location from the L-shaped bend can be problematic. Cases BS and BIO do not show much difference in their behavior of passing the posterior cavernous genu ICA, and cases BIM and BL show even less difference because of their longer inlet lengths and the rapid decay of the Womersley profile with the development of the secondary flow structure. Moreover, velocity distributions do not show any significant difference within two to three diameters downstream, which explains the insensitivity of cases BS and BIO to the inlet boundary conditions. However, as the mean flow rate increases, similar discrepancy in their flows in the L-shaped bends is observed.

There have been many analytical and numerical studies for the flow in a curved pipe with either/both curvature and torsion [67, 146, 13, 147]. The flow in the supraclinoid ICA, however, is different from the flow in simple geometric pipes, because of the diverse topological variation of anatomy, diameter change, anatomical complexity of vessel wall. Fortunately, there seems to be remarkable flow characteristics which can be understood from studies of flow in curved pipes with different curvature and torsion. The differences between A and B models in the behavior of sensitivity can be explained from that perspective. Patient A’s blood vessels are smaller in the diameter and the radii of the curvature of two turning segments, namely posterior and anterior cavernous genu, are also smaller than those of patient B. The smaller vessel diameter makes the mean velocity and the Reynolds number larger for a given average VFR. Small radii of the turning segments also mean larger Dean numbers. In other words, patient A simulations were done at higher Reynolds
number and Dean number than the cases BL, BIO, BIM, and BS. When the average VFR increases, the Reynolds number increases as well and cases BIH and BLH began to show similar differences observed in cases AS and AL.

### 3.3 Effect of outflow conditions

#### 3.3.1 Geometry and numerical setup

Three subjects B, C, and D in Table 3.1 are used to test sensitivity to outlet pressure boundary conditions. In order to check sensitivity of flow instability ans WSS/pressure distribution in the supraclinoid ICA, outlet pressure boundary conditions are modified using RC-type boundary condition. More specifically, the flow rates at the outlets such as MCA, ACA, and PCoA are changed from those in constant pressure condition. “RC boundary condition”, a variant of Windkessel model relates the pressure with the flow rates through the differential equation $P(t) + RC \frac{dP(t)}{dt} = Q(t)R$, where $P(t)$, $R$, $C$, $Q(t)$ are the pressure at the boundary, the resistance, the capacitance, and the flow rate, respectively [58]. In RC-type boundary condition, we increase the downstream Resistance $R$ to reduce the flow rate at the outlet and vice versa. The changes in VFRs at the large arteries like ACA and MAC are ± 20-30 ml/min, equivalent to 10-30 % of mean VFR. VFRs in small arteries like PCoA and OA increase/decrease by factor of 5-6. With subjects B and C, flow instability and velocity fluctuations are compared, while with subject D, WSS/pressure distribution as well as velocity fluctuations are compared. The flow rates at the inlet for subjects B, C, and D are 350 ml/min, 150 ml/min, and 300 ml/min, respectively; inlets are located in the ICA. These flow rates are chosen to induce instability in the flow, which will be discussed in detail at later chapter 6.

#### 3.3.2 Results

**Patient B**

Figure 3.8 shows quantitative changes in the flow when flow rates at the outlets flow change by a factor of 5 in small arteries and by 20 % in large outlets of patient B. Specifically, using RC boundary conditions, the flow rates at the PCoA and the ophtalmic artery is reduced by factor of 5, and the increase in MCA flow rate compensates the flow reduction in the
small arteries. The velocity time traces at the upstream and downstream history points are plotted and compared between constant pressure (CP) and RC-type (RC) outflow boundary condition. Velocity at more points are examined as well as the points in Figure 3.8. The zoom-in plots of time traces at ‘Pt’ 11, 15, and 18 show that the frequencies of small fluctuations does not change although the magnitudes of fluctuation change somewhat at some history points. The peak at ‘Pt’ 1 seems to disappear due to the flow rate increase in the MCA. However, the flow rate changes seem not to affect the flow instability.

**Patient C**

Figure 3.9 shows flow rate changes in the MCA/ACA. In this case, we apply two different RC boundary conditions, one of which (RC1) makes the flow rates close to those corresponding to the constant pressure condition. By imposing the other RC outflow boundary (RC2) condition, we increase the VFR at the MCA and reduce the flow at the ACA by 30%. Upstream history points do not show any high frequency oscillations seen in velocity time traces at history points inside the aneurysms. Velocity time traces at history points inside the aneurysms and upstream of aneurysms are almost the same among the different boundary conditions. Those downstream of the aneurysms show different magnitudes but similar fluctuations. Hence, we conclude that outlet flow rates does not seem to affect aneurysmal flow instability.

**Patient D**

Figures 3.10 and 3.11 show both qualitative and quantitative changes in the flow when different boundary conditions are employed. Specifically, three different boundary conditions are tested: constant pressure (CP), RC-type 1 (RC1), RC-type 2 (RC2). A large resistance, ‘R’ parameter, in RC1 and RC2 is used to reduce the VFR at the PCoA. RC1 and RC2 are set to induce large changes in the flow both in the MCA and in the ACA.

Qualitative distributions of WSS and pressure are virtually the same as shown in Fig. 3.10, except near the outlets and at the tip of the infundibulum. A pattern of a region of locally elevated pressure surrounded by a band of higher WSS is clearly seen in all three cases. High VFR at the PCoA under the CP condition creates extremely high WSS, which seems to be physiologically unreasonable. Imposing RC outflow boundary conditions reduces the VFR at the PCoA by a factor of six, while the $y$-component of velocity at ‘Pt’
Table 3.4: RC boundary conditions and flow rate change at the outlets. Outlets are numbered as shown in Figure 3.12.

<table>
<thead>
<tr>
<th>Outlet No.</th>
<th>R1</th>
<th>C1</th>
<th>R2</th>
<th>C2</th>
<th>F1</th>
<th>F2</th>
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<tr>
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<td>25</td>
<td>0.008</td>
<td>1.5</td>
<td>0.067</td>
<td>20.52826</td>
<td>21.967576</td>
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<tr>
<td>6</td>
<td>25</td>
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<td>2</td>
<td>0.05</td>
<td>24.093862</td>
<td>25.572252</td>
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<tr>
<td>7</td>
<td>40</td>
<td>0.005</td>
<td>12.5</td>
<td>0.008</td>
<td>10.147867</td>
<td>9.777337</td>
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<tr>
<td>8</td>
<td>100</td>
<td>0.002</td>
<td>200</td>
<td>0.0005</td>
<td>2.729854</td>
<td>1.277245</td>
</tr>
<tr>
<td>9</td>
<td>100</td>
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<td>200</td>
<td>0.0005</td>
<td>2.767650</td>
<td>1.274129</td>
</tr>
<tr>
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<td>100</td>
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<td>600</td>
<td>0.00017</td>
<td>2.269136</td>
<td>0.416875</td>
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<tr>
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<td>50</td>
<td>0.002</td>
<td>5.553003</td>
<td>4.995965</td>
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<tr>
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<td>50</td>
<td>0.004</td>
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<td>19</td>
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</tr>
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<td>100</td>
<td>0.001</td>
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<td>0.0033</td>
<td>4.594933</td>
<td>4.967349</td>
</tr>
</tbody>
</table>

10 near the tip of the infundibulum is reduced by a factor of three. However, flow rate changes in the MCA and the ACA via different ‘R’s in RC1 and RC2 conditions do not affect the velocity at the five history points shown in Fig. 3.11. The velocity at ‘Pt’ 43 near the aneurysm, which is located at the far upstream of the infundibulum, does not show any differences among the different cases as clearly shown in Fig. 3.11. Moreover, using constant pressure and lower VFR at the PCoA does not affect the velocity fluctuation.

Flow in the Circle of Willis

We test blood flow in the Circle of Willis and the VAs and ICAs harboring an aneurysm on the right hand side of the circulation. The RC boundary conditions are adjusted from $R_1$ and $C_1$ to $R_2$ and $C_2$ in order to see the sensitivity of aneurysmal flow to outflow boundary condition and to take the areas of outlets into account. If an outlet area is smaller and the resistance at the corresponding outlet is set to higher than outlets with larger cross-sectional areas. More detailed information are presented in chapter 6. Table 3.4 summarizes the changes in flow rates at the outlets in response to RC boundary condition changes with the outlets numbered as in Figure 3.13.
Figure 3.12 illustrates the changes in the velocity distribution in the planes marked in the inset geometry. There is no noticeable difference between the two cases although flow rates at the outlets changes by 20 % - 200 %, for example, from 5.6 to 8.4 in the right MCA outlet labeled as 14. Moreover, the ophtalmic artery with label 9 on the right is decreased from 2.7 to 1.27. Hence, the flow rate in the parent vessel of the aneurysm increases from 24.09 to 25.57 slightly. However, it does not affect the velocity distribution at all.

## 3.4 Resolution studies (‘hp-refinement’ test)

We perform a systematic ‘hp-refinement’ test under the same conditions used for our simulations. The time-dependent flow at the anatomically correct geometric model is tested at four different polynomial orders and four different meshes at fixed polynomial order $p=4$. This study is intended to make sure that the oscillation is not due to numerical artifacts caused by under-resolution and to confirm that our NEKTAR code can resolve high frequency oscillation caused by the hydrodynamic instability. Hence, we selected a case in which the velocity oscillates during the decelerating systole.

We used patient C’s two-aneurysm model. This geometric model was chosen because our study showed that the flow in the two adjacent aneurysms are prone to become unstable. The type of element used for space discretization is tetrahedral. For p-refinement test, the tested polynomial orders are $p = 4, 6, 8, 10$ and the grid points used in the calculations are $(p + 3)(p + 2)^2 = 252, 576, 1100, 1872$ per element, respectively. Since the total number of elements is 89324, the total grid points per variable for polynomial order $p = 10$ is 167,214,528. The effective distance between grid points in this case is about 0.0091 - 0.0364 mm in the aneurysm, which is 110 - 440 times smaller than the diameter of the inlet. For h-refinement, the number of elements are 81162, 103693, and 121807 with a polynomial order 4 and the reference was taken from the simulation with the largest number of elements 121807 and a higher order of polynomial ‘$p = 6$’.

### h-refinement

We checked convergence in the simulation using specific metric: the temporal average of spatial $L_2$ error in WSS against the results from a simulation with the finest mesh as a reference using equation (3.1). The frequency spectra of pointwise velocity are also compared
among the results from different meshes.

The formula for the WSS error calculation is defined as

\[ WSS_e = \frac{1}{N} \sum_{i=0}^{N-1} \left( \frac{\int |WSS_i - \tilde{WSS}_i|^2 dS}{\int dS} \right)^{1/2}, \]  

where the surface integration is done on the curved surface by numerical quadrature and the reference WSS \((p = 6, \text{number of elements 121K})\) is denoted by \(\tilde{WSS}\).

The frequency spectra are obtained from the time traces at history points close to the points used in p-refinement test shown in Figure 6.6 (left) and a point in the upstream parent vessel during the entire third cardiac cycle. The WSS distribution on a patch shown in Figure 3.14 (a) is calculated from the velocity field during the entire third cycle.

**p-refinement**

We checked convergence in the simulation using two metrics: the \(L_2\) error in time of point-wise velocity and temporal average of spatial \(L_2\) error in WSS. The errors are compared against the results from a simulation with the highest order polynomial, i.e. \(p = 10\), as a reference.

Simulations for error computations start from the systolic peak and continue until the dicrotic peak for the aforementioned reasons. This time interval for error computation is about 1/6 of the cardiac cycle as indicated by the red box in Figure 6.6.

The history points and the time interval during which temporal averages were taken are shown in Figure 6.6 (left and right, respectively.) A patch on which WSS errors are computed is shown in Figure 3.14 (a). The formula for WSS error calculation is equation (3.1), where the surface integration is done on the curved surface by numerical quadrature and the reference WSS \((p = 10)\) is denoted by \(\tilde{WSS}\). The velocity error at each history point is taken as

\[ V_e = \left( \frac{\sum_{i=0}^{N-1} |V_i - \tilde{V}_i|^2}{\sum_{i=0}^{N-1} |V_i|^2} \right)^{1/2}, \]  

where the reference velocity \((p = 10)\) is denoted by \(\tilde{V}\).

We performed a simulation with polynomial order \(p = 6\) up to four cardiac cycles. During the last cycle, the check points files were saved every time unit with time step \(\Delta t = 0.00025\). Using the check point file at the systolic peak of the fourth cycle, three more
simulations with different polynomial orders, i.e. \( p = 4, 8, \) and \( 10 \), were performed with the same time step, which satisfies the CFL condition for all polynomial orders.

### 3.4.1 Results

**h-refinement**

The \( L_2 \) errors of WSS from the h-refinement test show linear convergence over the size of element edge or the number of elements as shown in Figure 3.14 (b) and (c). Spectra from different meshes show similar peaks and the changes are insignificant among them as shown in Figure 3.14 (d).

**p-refinement**

Time traces of velocity at two history points are plotted in Figure 3.14 (f) showing no discernible difference. The \( L_2 \) errors of WSS and velocity from the p-refinement test show exponential convergence over the order of polynomial as shown in Figure 3.14 (g) and (h), respectively. Average WSS over the patch is about 10 \( N/m^2 \) and the error changes from 0.2956 \( N/m^2 \) (p=6) to 0.0591 \( N/m^2 \) (p=8). Hence, they are about 3 % and 0.6 % of average WSS. For velocity, errors are even smaller 0.1 % (p=6) and 0.01 % (p=8). WSS has one order lower accuracy because WSS is calculated through differentiation of field variables.

### 3.5 Conclusions

Sensitivity study shows that WSS distribution in aneurysms can be very sensitive to the inlet boundary condition. Wide-necked aneurysms and high VFRs create more sensitive flow than a narrow-necked case and low VFRs. However, WSS/pressure distribution and velocity fluctuations are less sensitive or insensitive to outflow boundary conditions if the region of interest is far (approximately 2 ~ 3 diameters upstream in our cases) from the bifurcation. The regions where changes are more noticeable are localized near the bifurcation and close to branches. VFRs at the small branches are changed by factor of 5-6 and those at the large downstream arteries such as MCA and ACA are by 10-30 %. WSS/pressure distribution, and velocity fluctuations are not sensitive to outflow rate changes.

Simulations with patient B geometry at VFR = 200 \( ml/min \) show no substantial difference in velocity or wall shear stress over the entire cardiac cycle. For the same VFR, 200 \( ml/min \), patient A models respond very sensitively to the inlet length variations. The
SAWSS between short and long models shows 60% differences in magnitude. In patient C models, the upstream aneurysm does not show any significant difference in SAWSS traces. On the patches of downstream aneurysm, however, SAWSSs demonstrate up to 100% difference between short and long model. When the VFR increases in cases of patient B, the SAWSS deviates between ‘short’ and ‘long’ models, resulting in 30% difference in magnitude. Overall, the difference between ‘intermediate’ and ‘long’ model is much smaller than the difference between ‘short’ and ‘long’ model. Hence, aneurysmal flow simulation should consider VFR and the presence of an aneurysm to avoid the entrance effect of simplified inlet boundary condition. For the simulations for aneurysmal flow near the supraclinoid ICA, imposing the inlet boundary condition at a location upstream of the lacerum ICA segment seems to give stable results.

hp-refinement study confirms that flow instabilities observed in the simulations of flow in patient-specific supraclinoid aneurysm and the circle of Willis are not numerical artifacts. Systematic and thorough simulations with mesh refinement and high-order polynomials shows the spectral convergence not only in velocity but also in WSS distribution.
Figure 3.1: Geometric models of patients A (left), B (middle), and C (right) in Table 3.1. Pink lines in the ICA show the locations of inlet boundary condition for short, intermediate, and long models. The short, intermediate, and long models include the cavernous segment, lacerum, and petrous ICA segment, respectively, as annotated in the center. Bottom row shows zoom-in of aneurysms indicated by blue circles in top row. The blue lines indicate the center of the supraclinoid ICA segment, which is the region of interest in this study, harboring aneurysms in patients A, B, and C.
Figure 3.2: (a) Volumetric flow rate (VFR) versus time at the inlet boundary. (b) $x$- (c) $y$- (d) $z$- component of velocity one diameter downstream from the numerical inlet boundary
Figure 3.3: (a)-(g): Spatially-averaged WSS versus time on the chosen patches among shown ones in (h) and pink arrows indicate corresponding patches used for spatial integration of viscous stress. Solid lines with circles and inverted triangles correspond to case AS and AL, respectively. * denotes the patches on the back of aneurysm.
Figure 3.4: (a)-(e): Spatially-averaged WSS versus time on the patches shown in (f) in cases BLH and BIH. Solid lines with circles and triangles correspond to case BLH and BIH, respectively. Average VFR is 300 ml/min and the average Reynolds numbers at the inlet are 353 and 381 for BLH and BIH.
Figure 3.5: (a)-(h): Spatially-averaged WSS on the patches shown in (i) in cases CS, CI, and CL. Solid lines with circles and triangles correspond to case CS and CL, respectively. Average VFR is 200 ml/min and the average Reynolds numbers at the inlet are 223, 255, and 253 for CL, CI, and CS, respectively.
Figure 3.6: Contour plot of WSS magnitude of patient A short vessel model (a) and patient A long vessel model (b) at the time shown in the inset (systolic peak). Top (bottom) row is a left (right) anterior oblique view of the aneurysm on the left supraclinoid ICA.
Figure 3.7: Isosurfaces and contours of velocity for the four cases (a) AS, (b) AI, (c) AL, (d) AM. Arrows indicate the general directions of the high velocity region. Circles indicate the part of isosurfaces which are located inside the aneurysm.
Figure 3.8: Patient B (VFR = 350 mL/min): Velocity time traces at history points with VFRs at the PCoA and the ophthalmic artery and the MCA over the cardiac cycle at different outflow boundary conditions. Black solid and red dotted lines correspond to constant pressure and RC-type outflow boundary conditions, respectively. Pt 5 is upstream of the aneurysm. Pt 1, 3, and 6 are downstream of the aneurysm. All other points are inside the aneurysm. X(L), Y(P), and Z(S) refer to lateral, posterior, and superior directions, respectively. ‘RC’ and ‘CP’ refer to RC-type and constant pressure outflow boundary conditions, respectively.
Figure 3.9: Patient C (VFR = 150 mL/min): Comparison of velocity time traces at history points upstream and downstream of the aneurysms among different outflow boundary conditions. Velocity time traces at the upstream history points show that the upstream flow is stable over the cardiac cycle and instability occurs in the aneurysms. Pink boxes on the some plots are showing zoom-in area. ‘RC1’, ‘RC2’, and ‘CP’ refer to RC-type 1, RC-type 2 and constant pressure outflow boundary conditions, respectively.
Figure 3.10: Patient D (VFR = 300 ml/min): Boundary condition effect on WSS, pressure, and flow rates in the Patient A at average VFR 300 ml/min. Peak VFRs under constant pressure, RC1, and RC2 conditions are (30.1, 5.1, 5.5 ml/min at the peak) in the PCoA, (207.1, 229.7, 249.6 ml/min at the peak) in the MCA, (180.3, 180.9, 160.7 ml/min at the peak) in the ACA.
Figure 3.11: Patient D (VFR = 300 ml/min) : Boundary condition effect on velocity at history points near the infundibulum of Patient D with VFR 300 ml/min. CP, RC1, and RC2 refer to constant pressure, RC-type 1, and RC-type 2.
Figure 3.12: Geometry of the circle of Willis for outflow boundary sensitivity and numbers of the outlets for Table 3.4.
Figure 3.13: u,v,w velocity contours on planes cutting ICA upstream and downstream of the aneurysm at a time instants marked in a left bottom plot.
Figure 3.14: (a) A patch where WSS errors are computed in reference to the highest polynomial order simulation ($p = 10$) or the finest mesh with higher order ($p = 6$). Colors on the patch in the upstream aneurysm represent the $x$ component of WSS vector at the systolic peak. (b) Plot of WSS $L_2$ error at the patch, which covers the upstream aneurysm walls, versus the largest edge length. (c) Plot of WSS $L_2$ error versus the number of elements. (d) the spectra at a history point inside the upstream aneurysm at different meshes. (e) Velocity time traces at history point Pt 1 inside the upstream aneurysm from four simulations with different polynomial order $p = 4, 6, 8$, and 10. (f) Velocity time traces at history point Pt 10 inside the downstream aneurysm from four simulations with different polynomial order $p = 4, 6, 8$, and 10. The differences between them, however, are not visually discernible. (g) $p$-convergence of $L_2$ error in WSS at the patch, which covers the upstream aneurysm walls, shown on the left during the time interval indicated with a red box in Figure 6.6. (h) $L_2$ error of pointwise velocity at several history points shows spectral (exponential) convergence.
Chapter 4

Solvers for the Navier-Stokes Equations

4.1 Introduction

Semi-implicit schemes are often used to solve advection-diffusion equations [70], where advection terms are nonlinear in general and diffusion terms are linear but stiff. Hence, nonlinear terms are solved explicitly to avoid Newton-Raphson type iteration and stiff linear diffusion terms are handled implicitly to avoid strict time step restriction. They are also referred to as implicit-explicit schemes (IMEX). For the Navier-Stokes equation, a high-order semi-implicit scheme was introduced with more accurate pressure boundary condition in [76], where the stiffly-stable scheme was employed to increase the stability regions. The nonlinear terms are treated explicitly and extrapolated in time for higher accuracy. The linear viscous terms are incorporated into the pressure boundary condition in the form of curl of the vorticity instead of Laplacian of velocity. The nonlinear term in the pressure boundary condition is also extrapolated in time to satisfy the compatibility condition of the pressure Poisson equation. In this chapter, we call this scheme in [76] the standard method.

The semi-implicit schemes in general have many advantages in efficiency compared to fully-implicit or fully-explicit methods. Moreover, the high-order temporal accuracy of the standard method has been exploited in many simulations from low to high Reynolds number flows [77]. However, the semi-implicit schemes based on the spectral method for spatial discretization over-resolve solutions in time due to large eigenvalues of the advection
operator which scales as $O(N^2)$, where $N$ is either the number of collocation points or the
order of polynomial basis. The CFL condition in the spectral method restricts $\Delta t$ which
scales like $O(1/N^2)$ when the solution to a hyperbolic equation is approximated with $N$
collocation points [55]. In the same token, time steps in the spectral element method also
scales as $O(1/N^2)$. Leriche et al. analyzed the stability of the standard scheme using
the eigenvalue analysis of Stokes equation [87]. Even for the Stokes problem, the scheme
is conditionally stable and the time step $\Delta t$ scales as $\Delta t < O(N^{-4})$ due to the explicit
treatment of the viscous term in the pressure boundary condition (the expansion order
$J_p \geq 3$). Hence, for the Navier-Stokes equation, the time restriction is solely from the
explicit nonlinear (convective) term, which scales like $O(1/N^2)$, only when the expansion
order $J_p \leq 2$.

Such overresolution in time increases prohibitively the computation time for large scale
simulations and particularly in pulsatile flows. In simulations of pulsatile flows, the time
step depends on the maximum velocity at the systolic peak. Hence, for the most of the
cardiac cycle, small time steps fixed for the systolic peak may be too small during the most
of cardiac cycle time, because the flow rates are much lower than that in the systolic peak.
In this study, we propose a simple method of sub-iteration to enhance the stability of the
semi-implicit scheme by suppressing the instability from the explicit expansion in pressure
boundary condition and by getting around the CFL condition.

Methods for alleviating the small time step problem include semi-Lagrangian temporal
discretization [114, 145] and fully-implicit treatment of the nonlinear convective acceleration
term [12]. Xiu et al. apply the semi-Lagrangian temporal method to spectral element
method [145]. Fixed-point iteration with Aitken relaxation was introduced in [72] and
has been used to update the position of the fluid-structure interface in the fluid structure
interaction simulations [99, 15, 82]. In this study, this is used as a way to stabilize the semi-
implicit spectral element methods. We show that sub-iteration with relaxation reduces the
divergence error at the boundary resulting in more accurate pressure boundary condition.
Moreover, the nonlinear convective term is calculated more accurately. Fixed-point itera-
tions are also used to solve the linearized steady Navier-Stokes equations. Employing the
spectral element method for the fluid structure interaction can be troublesome, because
small time steps tend to destabilize the fluid-structure interaction [82]. Hence, the spectral
element method we propose in this study is stable at large CFL flow conditions and can be
more readily applicable to fluid-structure interaction in a partitioned way.

This chapter is organized as follows. In section 4.2 we briefly describe the governing equations with boundary conditions and underlying assumptions followed by a new scheme for the Navier-Stokes equations based on the semi-implicit spectral/hp element method and eigenvalue analysis of our scheme. Accuracy test of our scheme with steady flows and unsteady flows appears in sections 4.3 and 4.4, respectively. A comparative study among the standard method, our sub-iteration scheme, and fully implicit scheme is also shown in section 4.3. We draw conclusions in section 4.5.

4.2 Governing equations and semi-discrete forms

In this section, we review the high-order semi-implicit method first proposed in [76] and analyzed in [61]. We consider the semi-discrete form of the Navier-Stokes equations which govern flows of incompressible and Newtonian fluid, i.e.,

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f} \quad \text{in } \Omega \\
\nabla \cdot \mathbf{u} = 0,
\]

where \( \mathbf{u} \) is the velocity vector, \( p \) the pressure, and \( \nu \) is the kinematic viscosity. An initial condition is given as \( \mathbf{u}(x, t = 0) = \mathbf{u}_0(x) \). On the boundary \( \partial \Omega \), either Dirichlet \( \mathbf{u}(x, t) = \mathbf{u}_D(x, t) \) or Neumann \( \partial \mathbf{u}(x, t)/\partial n = \mathbf{u}_N(x, t) \) is given.

Using the splitting scheme, the semi-discrete form of the Navier-Stokes equations is given as follows. Let \( \mathbf{u}^n \) denote an approximation of \( \mathbf{u} \) at time \( t = n \times \Delta t \). For numerical solutions given by the previous time steps solutions \( \mathbf{u}^{n-q} q = 0, ..., J-1 \), we solve the equations (4.2a) and (4.2b) for \( \mathbf{u}^{n+1} \) and \( p^{n+1} \).

\[
\frac{\hat{\mathbf{u}} - \sum_{q=0}^{J-1} \alpha_q \mathbf{u}^{n-q}}{\Delta t} = -\sum_{q=0}^{J-1} \beta_q [\mathbf{u} \cdot \nabla \mathbf{u}]^{n-q} - \nabla p^{n+1} \quad \text{with } \nabla \cdot \hat{\mathbf{u}} = 0, \\
\frac{\gamma \mathbf{u}^{n+1} - \hat{\mathbf{u}}}{\Delta t} = \nu \nabla^2 \mathbf{u}^{n+1},
\]
for the first sub-iteration with the following pressure boundary condition:

\[
\frac{\partial p^{n+1}}{\partial n} = \left[ \frac{\partial u^{n+1}}{\partial t} + \nu \sum_{q=0}^{J_p-1} \beta_q (\nabla \times \omega)^{n-q} + \sum_{q=0}^{J_e-1} \beta_q (u \cdot \nabla u)^{n-q} \right] \cdot n. \tag{4.3}
\]

The coefficients \(\alpha_i\), \(\beta_i\), and \(\gamma\) are given in table 4 of [76]. Here, \(J_i\), \(J_e\), and \(J_p\) denote the order of backward difference formula (BDF), explicit expansion of nonlinear term, and explicit expansion of viscous term, respectively. In this study, we use the same order for \(J_i\), \(J_e\), \(J_p\), and \(J\) denotes the order unless stated otherwise. The pressure Poisson equation is derived by taking the divergence of equation (4.2a) and applying incompressibility on the intermediate velocity field, \(\hat{u}\). Each component of velocity \(u^{n+1}\) in equation (4.2b) can be solved with a Helmholtz solver with Dirichlet or Neumann boundary condition. This Poisson equation and the three Helmholtz equations are discretized spatially using the spectral element method. The geometry of each element and unknown variables are represented with Jacobi polynomial basis. For more details of this method, we refer the reader to [77]. In this paper, we refer to this method as the “standard method”. For notational simplicity, we will denote the nonlinear term as \(N^{n-q} = u^{n-q} \cdot \nabla u^{n-q}\).

Accuracy and stability properties of the semi-implicit spectral element method are analyzed in [87]. We note that using one order less for \(J_p\) than \(J_i\) does not affect the temporal accuracy of the solution. Leriche et al. showed that a steady Stokes solver using the standard method is only conditionally stable when \(J_p\) is greater than 2, limiting the time step \(\Delta t < O(N^{-4})\), where the \(N\) is the order of polynomial space due to the explicit treatment of the pressure boundary condition. In Navier-Stokes solvers with explicit nonlinear (convective) term, the time step \(\Delta t\) is solely restricted by the CFL condition and scales likes \(O(1/N^2)\), although \(J_p \leq 2\) is used. Hence, we propose a method which is not restricted by the CFL conditions while the nonlinear term is still treated explicitly. This is important from the computational standpoint as we end up with a solution of a symmetric linear system for which effective preconditioners exist [59, 120].

### 4.2.1 Sub-iteration of semi-implicit scheme

This solver employs the high-order splitting scheme and each time step consists of sub-iterations which continue until the \(L_{\infty}\) norm of velocity and pressure field difference between two subsequent substeps becomes smaller than a given tolerance. We introduce a
sub-iteration scheme which updates the nonlinear term. When the explicit nonlinear term
is updated, the pressure boundary condition must be set accordingly to satisfy the com-
patibility condition of the Poisson equation for the pressure. At the first sub-iteration step
\( k = 1 \), for given previous time step solutions \( u^{n-q}, q = 0, ..., J - 1 \) we solve equations
(4.2a) and (4.2b) for \( u^{n+1}, p^{n+1} \) with the pressure boundary condition in (4.3). This so-
lution \( (u^{n+1}, p^{n+1}) \) is set to the first sub-iteration step solution \( u_1^{n+1}, p_1^{n+1} \) for the next sub-iteration step.

From the second sub-iteration step \( k (\geq 2) \), the nonlinear term \( N_{n+1}^{k-1} = u_{k-1}^{n+1} \cdot \nabla u_{k-1}^{n+1} \)
can be computed using previous sub-iteration step solutions \( u_{k-1}^{n+1} \) and \( p_{k-1}^{n+1} \) instead of
time extrapolation. The pressure boundary condition that contains the viscous term, i.e.
\((\nabla \times \omega)^{n+1}_{k-1}\), is handled similarly. Hence the following equations (4.4a)-(4.4b) are used from
the second sub-iteration, \( k \geq 2 \):

\[
\begin{align*}
\hat{u} - \sum_{q=0}^{J-1} \alpha_q u^{n-q} \frac{\Delta t}{\Delta t} &= -N_{k-1}^{n+1} - \nabla P_{k}^{n+1}, \quad (4.4a) \\
\gamma u_{k}^{n+1} - \hat{u} \frac{\Delta t}{\Delta t} &= \nu \nabla^2 u_{k}^{n+1}, \quad (4.4b)
\end{align*}
\]

with the following pressure boundary condition at the sub-iteration step \( k \):

\[
\frac{\partial P_{k}^{n+1}}{\partial n} = - \left[ \frac{\partial u_{k}^{n+1}}{\partial t} + \nu (\nabla \times \omega)^{n+1}_{k-1} + N_{k-1}^{n+1} \right] \cdot n. \quad (4.5)
\]

At the end of each sub-iteration step \( k \) of time level \( n+1 \), Aitken relaxation is employed
and the relaxation parameter \( \lambda^k \) at sub-iteration step \( k \) is updated every sub-iteration
through the following rule :

\[
\tilde{u}_{k+1}^{n+1} = \lambda_{k+1} \tilde{u}_{k}^{n+1} + (1 - \lambda_{k+1}) u_{k+1}^{n+1}. \quad (4.6)
\]

Here, \( \lambda_k \) is updated through the following Aitken scheme:

\[
\lambda_{k+1} = \lambda_k + (\lambda_k - 1) \frac{(Q_k - Q_{k+1}) \cdot Q_{k+1}}{||Q_k - Q_{k+1}||^2}, \quad (4.7)
\]

where \( Q_{k+1} = \tilde{u}_{k}^{n+1} - u_{k+1}^{n+1} \) and \( u_{k+1}^{n+1} \) is the numerical solution from equations (4.4a) and
(4.4b). The calculated \( \lambda_{k+1} \) is limited to be in \([\lambda_{min}, \lambda_{max}]\) by setting a closest value when
the calculated $\lambda$ is outside of the range. In this study, $\lambda_{min} = 0.0$, and $\lambda_{max} = 0.9$ are used unless stated otherwise. The sub-iteration stops and the algorithm continues to the next time step level ($n+2$) if both $|u^{n+1}_k - u^{n+1}_{k-1}|_{\infty}$ and $|p^{n+1}_k - p^{n+1}_{k-1}|_{\infty}$ are less than a tolerance, e.g. $10^{-6}$ or $10^{-7}$. We also confirmed that a larger tolerance in the order of $10^{-3}$ or $10^{-4}$ can be used for speedup, but at the cost of a slight loss of accuracy.

4.2.2 Eigenvalue analysis of the Stokes equations

We analyze the stability of the new method for the Stokes equations when $J_p = 3$ following [87] because the standard method is shown to be unconditionally stable for $J_p \leq 2$, but becomes unstable at large $\Delta t$ for $J_p = 3$. For eigenvalues of the evolution operators, the Stokes equations are discretized in time as in equations (4.2a) - (4.3) for the standard method and equations (4.4a)-(4.5) for our new scheme. A body force is not considered in this analysis. The numerical domain is $[-1, 1] \times [-1, 1]$ and the equations are spatially discretized with the Chebyshev collocation method of order $N = 12$ or higher. Homogeneous Dirichlet boundary conditions for velocity and Neumann pressure boundary conditions are applied in all boundaries of the domain. Then, a matrix which takes into account the Neumann pressure boundary condition and BDF is generated and the eigenvalues are obtained.

At five different $\Delta t = 0.001, 0.05, 1, 100,$ and $1000$, the leading eigenvalues are obtained as shown in Table 4.1. As Leriche et al. reported, the 3rd-order standard scheme becomes unstable for large $\Delta t$ above 0.001 in our particular case and the leading eigenvalues are larger than a unit. The magnitude of leading eigenvalues at $\Delta t = 100$ and 1000 are close to 1.153 reported in [87]. The stabilizing effect of sub-iteration is clearly shown in that sub-iterations decrease the magnitude of the leading eigenvalue from 1.1311 to 0.8726 and from 1.1051 to 0.7545 for $\Delta t = 100$ and $\Delta t = 0.05$, respectively. For small $\Delta t$ (< 0.001), the approximate solution at the first sub-iteration step is already accurate enough and many sub-iterations are not needed for corrections. Consequently, sub-iterations do not change the eigenvalues. However, for large $\Delta t$, the solutions take tens of sub-iterations to reach accurate solution at the next time level and then leading eigenvalues stop changing. For example, the leading eigenvalue of the evolution operator at $\Delta t = 0.05$ does not change from sub-iteration step 10, but the corresponding eigenvalue at $\Delta t = 1$ decrease until sub-iteration step 20.

The discrete evolution operator is advancing the solution at time step $n, n-1, ..., n-J+1$ to an approximate solution at time step $n+1$. Without any body force or energy flux through
the boundary, the energy in the system should decay due to viscosity. Hence we expect that
the largest eigenvalue for small $\Delta t$ and large $\Delta t$ is close to 1 and 0, if the evolution operator is
accurate. The discrete evolution operator of our scheme is more accurate and the magnitude
of leading eigenvalues decreases as the time step increases, which mimics the viscous decay
of energy of eigen modes. As the eigenvalue analysis of sub-iteration scheme shows, our
method is numerically confirmed to be stable at $\Delta t$ 100 or 1000 when the simulations start
from the exact solutions.

In order to demonstrate the change in location of the eigenvalues in the complex
plane visually, the eigenvalues of the evolution operator are plotted in the complex plane
with a unit circle in Figure 4.1 for two cases, $\Delta t = 0.05$ and 100. For $\Delta t \geq 0.001$, the
leading eigenvalue is larger than 1 and outside of the unit circle. Figure 4.1 (left) shows
the spectra of the evolution operator of the standard method without any sub-iteration and
some eigenvalues are outside of the unit circle. On the other hand, sub-iterations reduce the
magnitude and push the leading eigenvalues inside the unit circle. Sub-iteration does not
change the distribution pattern from the backward difference formula and they are always
inside the unit circle. Sub-iteration, however, scales down the eigenvalues outside of the
unit circle and make them stay inside the unit circle.

Table 4.1: Leading eigenvalues and their magnitudes of the evolution operator for the Stokes
equations with $N = 12$. One sub-iteration corresponds to the standard scheme.

<table>
<thead>
<tr>
<th>Iterations</th>
<th>1000</th>
<th>$\Delta t$</th>
<th>1.0</th>
<th>0.05</th>
<th>0.001</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>100</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>(0.846+0.750i)</td>
<td>(0.845+0.750i)</td>
<td>(0.834+0.759i)</td>
<td>(0.750+0.811i)</td>
<td>0.986</td>
</tr>
<tr>
<td></td>
<td>1.131</td>
<td>1.131</td>
<td>1.128</td>
<td>1.105</td>
<td>0.986</td>
</tr>
<tr>
<td>4</td>
<td>(0.285+0.824i)</td>
<td>(0.285+0.824i)</td>
<td>(0.160+0.756i)</td>
<td>(0.134+0.742i)</td>
<td>0.986</td>
</tr>
<tr>
<td></td>
<td>0.872</td>
<td>0.872</td>
<td>0.773</td>
<td>0.754</td>
<td>0.986</td>
</tr>
<tr>
<td>10</td>
<td>(-0.046+0.474i)</td>
<td>(0.003+0.583i)</td>
<td>(-0.055+0.451i)</td>
<td>(0.554+0i)</td>
<td>0.986</td>
</tr>
<tr>
<td></td>
<td>0.476</td>
<td>0.583</td>
<td>0.455</td>
<td>0.554</td>
<td>0.986</td>
</tr>
<tr>
<td>20</td>
<td>(-0.064+0.165i)</td>
<td>(-0.063+0.165i)</td>
<td>(-0.007+0.321i)</td>
<td>(0.554+0i)</td>
<td>0.986</td>
</tr>
<tr>
<td></td>
<td>0.177</td>
<td>0.176</td>
<td>0.321</td>
<td>0.554</td>
<td>0.986</td>
</tr>
<tr>
<td>25</td>
<td>(-0.045+0.100i)</td>
<td>(-0.045+0.100i)</td>
<td>(-0.007+0.321i)</td>
<td>(0.554+0i)</td>
<td>0.986</td>
</tr>
<tr>
<td></td>
<td>0.109</td>
<td>0.109</td>
<td>0.321</td>
<td>0.554</td>
<td>0.986</td>
</tr>
<tr>
<td>35</td>
<td>(-0.020+0.038i)</td>
<td>(-0.027+0.060i)</td>
<td>(-0.007+0.321i)</td>
<td>(0.554+0i)</td>
<td>0.986</td>
</tr>
<tr>
<td></td>
<td>0.0431</td>
<td>0.066</td>
<td>0.321</td>
<td>0.554</td>
<td>0.986</td>
</tr>
</tbody>
</table>
Figure 4.1: Spectra of the evolution operator of the standard scheme (left) and new scheme with sub-iteration (right). $\Delta t = 100.0$ (top) and $\Delta t = 0.05$ (bottom) and $J_i = J_p = 3$ and $N = 12$.

4.2.3 Fully-implicit solver

In order to evaluate the efficiencies of the sub-iteration scheme, we test it against a fully-implicit scheme proposed recently by Dong and Shen in [34]; our implementation here is slightly different. The first and second splitting steps that treat the nonlinear term and solves for pressure, respectively, are identical to the standard method in [76]. The third splitting step, velocity correction step, includes the $\hat{u} \cdot \nabla u^{n+1}$, where $\hat{u}$ indicates an estimate of velocity at time level $n + 1$.

\[
\frac{\hat{u} - \sum_{q=0}^{J_e-1} \alpha_q u^{n-q}}{\Delta t} = - \sum_{q=0}^{J_e-1} \beta_q [u \cdot \nabla u]^{n-q}, \tag{4.8a}
\]

\[
\frac{\hat{u} - \hat{\hat{u}}}{\Delta t} = -\nabla p^{n+1}, \tag{4.8b}
\]

\[
\frac{\gamma u^{n+1} - \hat{u}}{\Delta t} = \nu \nabla^2 u^{n+1} - \hat{u} \cdot \nabla u^{n+1} + \sum_{q=0}^{J_e-1} \beta_q [u \cdot \nabla u]^{n-q}. \tag{4.8c}
\]
Here, $\tilde{u}$ in the third splitting step, is given by

$$\tilde{u} = \sum_{q=0}^{J_n-1} \beta^q u^{n-q}, \tag{4.9}$$

where $J_n = 1$ or $2$. Dong and Shen estimate the convection velocity $\tilde{u}$ by including explicitly the linear viscous term in the form of curl of the vorticity in the first splitting step. In our implementation, we use the previous time step $u^n$ or time extrapolation. We present a comparative study of stability and accuracy between this fully implicit scheme and our sub-iteration scheme in section 4.4.2.

### 4.3 Numerical simulations: steady flow

Here we check stability and accuracy of the new scheme with exact solutions in steady flow cases. First, we confirm that our scheme solves the Navier-Stokes equations accurately and maintains stability at large time steps. With analytic steady solutions, i.e. Wannier and Kovasznay flows, we tested the convergence behavior of our scheme.

#### 4.3.1 Wannier flow

Wannier flow is a two-dimensional Stokes flow past a rotating cylinder near a moving wall [142]. In this test, a cylinder of radius $R = 0.25$ is located at the $(0,0)$ in a numerical domain $[-3,3] \times [-0.5,2.5]$. The parameters used in the simulation are the rotational velocity of the cylinder $\omega = 2.0$, the distance between the center of the rotating cylinder and the moving wall $d = 0.25$, and the velocity of the moving wall $U = 1.0$. Its exact solution is given as

$$u(x,y) = U - 2(a_1 + a_0 Y_1) \left[ \frac{s + Y_1}{K_1} + \frac{s - Y_1}{K_2} \right] - a_0 \ln(\frac{K_1}{K_2})$$

$$- \frac{a_2}{K_1} \left[ s + Y_2 - \frac{(s + Y_1)^2 Y_2}{K_1} \right]$$

$$- \frac{a_3}{K_2} \left[ s - Y_2 + \frac{(s - Y_1)^2 Y_2}{K_2} \right], \tag{4.10}$$

$$v(x,y) = \frac{2x}{K_1 K_2} (a_1 + a_0 Y_1)(K_2 - K_1) - \frac{xa_2(s + Y_1)Y_2}{K_1^2} - \frac{xa_3(s - Y_1)Y_2}{K_2^2}, \tag{4.11}$$
where the parameters are

\[ a_0 = \frac{U}{\ln(\Gamma)}, \quad b_0 = \frac{r^2 \omega}{2s} \]
\[ a_1 = -d(a_0 + b_0), \quad a_2 = 2(d + s)(a_0 + b_0), \quad a_3 = 2(d - s)(a_0 + b_0) \]
\[ Y_1 = y + d, \quad Y_2 = 2Y_1 \]
\[ K_1 = x^2 + (s + Y_1)^2, \quad K_2 = x^2 + (s - Y_1)^2. \] (4.12)

Figure 4.2: Triangular spectral elements \( (N_{el} = 137, \text{ polynomial order } p = 16) \) and streamlines around the rotating cylinder of Wannier flow.

The domain is spatially discretized with 137 spectral elements and the approximate solutions are represented with polynomial order 16 in each element. The spectral element mesh and streamlines are shown in Figure 4.2 (left) and (right), respectively. For the integration order \( (J = 3) \), the standard method becomes unstable at \( \Delta t > 10^{-3} \) in steady Stokes flow. We confirm numerically that our Stokes solver with sub-iterations is unconditionally stable at \( J = 3 \) as shown in the previous eigenvalue analysis. Sub-iteration with Aitken relaxation contributes to the stability of our scheme at large time steps, but does not improve the accuracy at steady state, because there is no time splitting error in solving steady flows. For \( J = 3 \), the \( L_2 \) error in Wannier flow is plotted against time step \( \Delta t \) in Figure 4.3. At \( \Delta t \) of \( O(1) \), the steady state errors increase slightly but are still in the order of \( O(10^{-7}) \). Even for \( \Delta t \geq 1 \), the \( L_2 \) errors of \( (u, v) \) do not increase but stay at the order of \( 10^{-6} \sim 10^{-7} \). For example \( \Delta t = 1000 \), the \( L_2 \) errors of \( (u, v) \) are \( 1.523e - 06 \) and \( 6.355e - 07 \), respectively.

Next, we address efficiency by checking the effect of sub-iterations on the error decay in Wannier flow by comparing cases in which only one or many sub-iterations (up to 20 sub-iterations) are allowed. The errors of the new scheme with many sub-iterations decay faster than in cases with only one sub-iteration for all integration orders \( J = 1, 2, \) and 3.
Figure 4.3: Plot of $L_2$ error versus time step, $\Delta t$ with polynomial order $p = 12$ and integration order $J = 3$ in both simulations of Wannier flow. The vertical dotted line shows the $\Delta t$, which the standard method becomes unstable due to the time explicit treatment of the pressure boundary condition.

Large time step $\Delta t$ tends to slow down the error decay as shown in Figures 4.4 (a) and (b). However, the sub-iteration scheme is less affected by such time step increase. For example, the $L_2$ error decays much slower when $\Delta t = 0.5$ is larger (Figure 4.4 (a-b) ) than $\Delta t = 0.1$ (Figure 4.4 (c-d)). Even at large time step $\Delta t = 0.5$, sub-iteration scheme reaches steady states within 6 time units, while one sub-iteration cases do not reach steady state until time units 15 and 30 for integration order $J=1$ and 2, respectively. Overall, $J = 1$ shows the fastest error decay while $J = 3$ shows the smallest steady state errors in all cases and then $J = 2$; however the difference among them is not significant.

4.3.2 Kovasznay Flow

Next, we check the stability of the sub-iteration scheme in solving the steady Navier-Stokes equations and make comparison against the implicit scheme with Kovasznay flow given in [80] as

$$u(x, y) = 1 - e^{\lambda \pi} \cos(2\pi y), \quad v(x, y) = \frac{\lambda}{2\pi} e^{\lambda x} \sin(2\pi y), \quad (4.13a)$$
where $\lambda = R/2 - \sqrt{R^2/4 + 4\pi^2}$ and $R$ denotes the Reynolds number. In this study, $R = 40$ is used and the numerical domain is $[-0.5, 1] \times [-0.5, 1.5]$. Dirichlet boundary conditions for velocity are specified on all sides of the domain and Neumann pressure boundary conditions are calculated from the velocity field. Meshes and streamlines are shown in Figure 4.5 (left).

For $J = 2$ and polynomial order $p = 14$, the standard method becomes unstable at $\Delta t = 0.01$, while our iterative scheme is stable and accurate above $\Delta t = 1.0$ with a slight degradation of steady state errors. The number of sub-iterations at each time step gradually decreases as it approaches the steady state solution.

Sub-iteration versus implicit scheme

We check the accuracy and stability of our sub-iteration scheme by comparing with implicit scheme (see equations (4.8a) - (4.8c)). Our implementation of fully implicit method is stable and accurate up to time step $\Delta t = 5$, while the sub-iteration scheme is stable and accurate up to $\Delta t = 3$ for integration order $J = 2$. Our implicit scheme becomes unstable above $\Delta t = 5$ as summarized in Table 4.2. As observed in the sub-iteration scheme, the steady state error of the implicit scheme increases gradually with time step $\Delta t$. In contrast, Dong and Shen’s implementation is unconditionally stable but the steady state errors suddenly
increase to above $O(10^{-1})$ around time step $\Delta t = 0.4$. The sub-iteration scheme also shows such a sudden increase above $O(1)$ in the steady state error, but it occurs at much larger time step $\Delta t = 2.0 \sim 3$. Much more dramatic results are from modification of the range of relaxation parameter from $(0, 0.9)$ to $(0, 0.99)$. In such case, the scheme seems to be unconditionally stable and accurate. For example, for $J_e = 2, 3$ and at $\Delta t = 1000$, steady state errors are in the order of $O(10^{-7})$.

Steady state errors at different time step $\Delta t$ in the Kovasznay flow are summarized in Table 4.2 for polynomial order $p = 12$. Here we use different integration order for $J_i, J_e$, and $J_n$, because $J_e$ affect the stability of the implicit scheme significantly. The stability of implicit scheme depends on $J_e$, the order of explicit nonlinear term in the pressure boundary condition. As $J_e$ increases from 1 to 2, the errors are reduced by order of 1 or 2. However, our implicit scheme becomes less stable and maximum time step decreases from 5 to $10^{-2}$ for both $J_i = 2, 3$ and regardless of the order $J_n$, time extrapolation of the convective velocity as listed in Table 4.2. We note that the order of $J_n$ for the linearized convection term affects the stability of the scheme slightly. The maximum time steps of the standard method for Kovasznay flow are listed for a better comparison. It is clear that the maximum size of time steps of implicit scheme with $J_e = 2$ are in the order of $10^{-2} \sim 10^{-3}$ close to those of the standard method.
Table 4.2: Kovasznay flow: Comparison of maximum time step $\Delta t$ and steady state errors in $(u,v)$ of Kovasznay flow between implicit scheme and the standard method. For larger time step $\Delta t$, schemes become unstable. Polynomial order $p = 12$ is used. * Range of relaxation parameter is modified to $[\lambda_{\text{min}}, \lambda_{\text{max}}] = (0.0, 0.99)$ while all other cases use $[\lambda_{\text{min}}, \lambda_{\text{max}}] = (0.0, 0.9)$.

<table>
<thead>
<tr>
<th>$(J_i, J_e, J_n)$</th>
<th>Implicit scheme</th>
<th>Sub-iteration method p = 12</th>
<th>Sub-iteration method* p = 12</th>
<th>Standard method p = 12</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(2,1,1)$</td>
<td>Max. $\Delta t$</td>
<td>$L_2$</td>
<td>$H_1$</td>
<td></td>
</tr>
<tr>
<td>$(2,1,2)$</td>
<td>5.0</td>
<td>(2.66e-07, 1.59e-07)</td>
<td>(1.48e-06, 1.67e-06)</td>
<td></td>
</tr>
<tr>
<td>$(3,1,1)$</td>
<td>5.0</td>
<td>(2.38e-07, 1.37e-07)</td>
<td>(1.32e-06, 1.48e-06)</td>
<td></td>
</tr>
<tr>
<td>$(3,1,2)$</td>
<td>4.0</td>
<td>(2.04e-07, 1.24e-07)</td>
<td>(1.28e-06, 1.38e-06)</td>
<td></td>
</tr>
<tr>
<td>$(2,2)$</td>
<td>$\Delta t$</td>
<td>$L_2$</td>
<td>$H_1$</td>
<td></td>
</tr>
<tr>
<td>$(2,2)$</td>
<td>2.0</td>
<td>(3.45e-07, 1.79e-07)</td>
<td>(2.13e-06, 2.00e-06)</td>
<td></td>
</tr>
<tr>
<td>$(3,3)$</td>
<td>1.0</td>
<td>(1.82e-07, 9.00e-08)</td>
<td>(1.28e-06, 1.13e-06)</td>
<td></td>
</tr>
<tr>
<td>$(3,3)$</td>
<td>2.0</td>
<td>(2.01e-01, 3.62e-01)</td>
<td>(2.06, 4.05)</td>
<td></td>
</tr>
<tr>
<td>$(2,2)$</td>
<td>1000</td>
<td>(9.70e-07, 7.37e-07)</td>
<td>(5.57e-06, 6.55e-06)</td>
<td></td>
</tr>
<tr>
<td>$(3,3)$</td>
<td>1000</td>
<td>(9.65e-07, 7.32e-07)</td>
<td>(5.54e-06, 6.51e-06)</td>
<td></td>
</tr>
</tbody>
</table>

Dependence on polynomial order $p$ and relaxation

We check the effect of polynomial order and relaxation on stability by changing the order of polynomial order $p$ and sub-iterating without relaxation. As the results are summarized in Table 4.3, the maximum time step $\Delta t$ of the sub-iteration scheme does not seem to be affected by order of polynomial $p$. Sub-iteration without relaxation becomes unstable at time step $\Delta ts$ which are comparable to those of the standard method. As observed in Kovasznay flow with $p = 12$, the change in the range of the relaxation parameter also demonstrates much more enhanced stability for $p = 16$. Regardless of $J_e$, the scheme is stable and accurate even at time step $\Delta t = 1000$ as the steady state errors are of order $O(10^{-9}) \sim O(10^{-10})$. 
Table 4.3: Kovasznay flow: Comparison of maximum time step $\Delta t$ and steady state errors in $(u,v)$ between sub-iteration scheme with and without relaxation, and between polynomial order $p = 12$ and $p = 16$. * Range of relaxation parameter is modified to $[\lambda_{\text{min}}, \lambda_{\text{max}}] = (0.0, 0.99)$ while all other cases use $[\lambda_{\text{min}}, \lambda_{\text{max}}] = (0.0, 0.9)$.

<table>
<thead>
<tr>
<th>Sub-iteration method $(J_i, J_e)$</th>
<th>Max. $\Delta t$</th>
<th>$L_2$</th>
<th>$H_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(2,2)$</td>
<td>2.0</td>
<td>(3.45e-07, 1.79e-07)</td>
</tr>
<tr>
<td></td>
<td>$(2,2)$</td>
<td>3.0</td>
<td>(2.34e-03, 8.00e-03)</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>1.0</td>
<td>(1.82e-07, 9.00e-08)</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>2.0</td>
<td>(2.01e-01, 3.62e-01)</td>
</tr>
<tr>
<td>Sub-iteration method $p = 16$</td>
<td>$(2,2)$</td>
<td>2.0</td>
<td>(1.37e-09, 4.25e-09)</td>
</tr>
<tr>
<td></td>
<td>$(2,2)$</td>
<td>3.0</td>
<td>(9.49e-04, 2.94e-03)</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>1.0</td>
<td>(7.05e-10, 2.47e-09)</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>2.0</td>
<td>(2.19e-01, 3.34e-01)</td>
</tr>
<tr>
<td>Sub-iteration method $^*$ $p = 16$</td>
<td>$(2,2)$</td>
<td>1000</td>
<td>(3.98e-09, 5.74e-09)</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>1000</td>
<td>(8.85e-10, 1.40e-09)</td>
</tr>
<tr>
<td>Sub-iteration method $p = 16$ (w/o) relaxation</td>
<td>$(2,2)$</td>
<td>0.02</td>
<td>(1.09e-10, 5.13e-10)</td>
</tr>
<tr>
<td></td>
<td>$(2,2)$</td>
<td>0.03</td>
<td>unstable</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>0.01</td>
<td>(3.00e-09, 3.35e-09)</td>
</tr>
<tr>
<td></td>
<td>$(3,3)$</td>
<td>0.02</td>
<td>unstable</td>
</tr>
</tbody>
</table>

4.3.3 Effect of sub-iteration on the divergence error

Preserving incompressibility of flow fields is a challenge in simulations of incompressible Newtonian flow, especially using splitting schemes. The divergence of the velocity field should be zero throughout the domain including boundaries. However, splitting of the Navier-Stokes equation into three decoupled equations and introduction of pressure boundary conditions create erroneous divergence error with more pronounced errors near the velocity Dirichlet boundaries. The analysis in [76] shows that the explicit extrapolation with $J_p$ time steps decreases the divergence error at the boundary by controlling the divergence flux which scales as $(\Delta t)^{J_p}$. Due to the divergence flux $\partial(\nabla \cdot u)/\partial n$, the divergence error at a boundary scales as $(\nu \Delta t)^{J_p}$. Hence, we check the effect of sub-iteration on the divergence error in Wannier flow and Kovasznay flow presented earlier.

First, we test the divergence errors in Wannier flow without any sub-iteration. Aitken
relaxation is performed at the end of each sub-iteration step. Due to the large time step $\Delta t = 0.5$, the errors are on the order of $O(1)$ at the bottom and near the rotating cylinder as shown in Figure 4.6. The relaxation reduces the divergence error slightly as shown in Figure 4.6. Changes from time step $n=5$ to $n=6$ is also negligible. Then, we check the distribution of divergence of the velocity field at every sub-iteration before and after the Aitken relaxation. Under the same flow conditions, Figure 4.7 shows the effect of sub-iterations on the divergence error in Wannier flow. At the same time step $n = 5$, sub-iterations have reduced the divergence error level down to $O(10^{-2}) \sim O(10^{-3})$ at the moving bottom boundary. Sub-iteration with relaxation reduces the divergence error at early sub-iteration steps $k=0$ and $k=1$ more effectively than later sub-iteration steps.

The divergence flux, $\frac{dQ}{dn} = \partial(\nabla \cdot u)/\partial n$, through the bottom wall in Wannier flow is plotted in Figure 4.8. As divergence error in the flow field decreases through the sub-iteration, the divergence flux also reduces significantly after the relaxation for the first couple of sub-iteration steps. From the second sub-iteration steps, the error is below 0.05 and flux errors are concentrated near the rotating cylinder at the bottom wall.
As in the steady Stokes flow, we also confirm that sub-iterations suppress divergence errors at the boundary in the steady Navier-Stokes flow. Using Kovasznay flow, the effect of sub-iteration on the divergence error ($\nabla \cdot \mathbf{u}$) and the divergence flux is measured, specifically, for $J = 3$ and $\Delta t = 0.5$ which makes the standard scheme unstable. The divergence error is as large as 0.18 on the left and right boundaries of the domain due to the large time step $\Delta t = 0.5$ during the first couple of sub-iteration. As the sub-iterations update the flow field, the velocity field becomes more accurate. Hence, the divergence error becomes much smaller. In the first sub-iteration, the relaxation decreases the divergence error significantly. In later sub-iteration steps, the changes are not as significant as in the first sub-iteration. The divergence flux, $\partial Q/\partial n$, is calculated near the right boundary of the numerical domain $[-0.5, 1] \times [-0.5, 1.5]$. The changes in the divergence flux are similar to that of divergence error.

### 4.3.4 Sub-iteration or relaxation?

Here, we analyze the effect of sub-iteration and relaxation on the stability of the scheme using a scalar linear advection-diffusion equation. Since it is shown that the sub-iteration stabilizes instability from the explicit expansion of viscous term in the pressure boundary condition, here we check the effect on the instability from the explicit advection term. To
that end, we consider a scalar linear convection-diffusion equation for analysis.

\[
\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} 
\] (4.14)

Suppose that the solution is periodic in space. Then the equation is discretized semi-implicitly in time as follows:

\[
\frac{\tilde{u}^{n+1} - \tilde{u}^n}{\Delta t} = -U i \omega \tilde{u}^n - \omega^2 \nu \tilde{u}^{n+1}, \\
\left[ \frac{1}{\Delta t} + \omega^2 \nu \right] \tilde{u}^{n+1} = U i \omega \tilde{u}^n - \frac{\tilde{u}^n}{\Delta t}.
\] (4.15) (4.16)

The scheme is stable if \( D_{sc} = |(\frac{1}{\Delta t} + U i \omega)/(\frac{1}{\Delta t} + \omega^2 \nu)| \leq 1 \) for all \( \omega \geq 0 \), which gives the range of \( \Delta t \leq 2 \nu / U^2 \). This is the time restriction in a semi-implicit scheme. For a given \( \Delta t \), the kinematic viscosity \( \nu \) should be larger than \( \Delta t c^2 / 2 \). Now, if the sub-iteration is introduced, then

\[
\left[ \frac{1}{\Delta t} + \omega^2 \nu \right] \tilde{u}_{k}^{n+1} = -U i \omega \tilde{u}_{k-1}^{n+1} + \tilde{u}_k^n, \\
\left[ \frac{1}{\Delta t} + \omega^2 \nu \right] \tilde{e}_{k}^{n+1} = -U i \omega \tilde{e}_{k-1}^{n+1}.
\] (4.17) (4.18)
The errors converge if the ratio

$$D_{su} = \frac{|U i \omega|}{1/\Delta t + \omega^2 \nu} \leq 1,$$

(4.19)

which gives a condition on time step $\Delta t \leq 4 \nu / U^2$. Hence the time step is enlarged by 2 times, but the stable time step $\Delta t$ for sub-iteration is still limited. This increased size of stable time step due to the effect of sub-iteration only is numerically confirmed with the comparison between cases with sub-iteration but without relaxation and cases without any sub-iteration (standard method). For example, for $p = 16$ maximum size of stable time step increases from 0.005 to 0.02, i.e by factor of 4 for $J_e = 2$. For $J_e = 3$, sub-iteration increases the maximum size of stable time step from 0.002 to 0.01 by factor of 5. Numerical simulations with the first-order scheme follow the analysis more closely. For $J_e = 1$, the maximum size of time step is 0.2 for sub-iteration scheme without relaxation compared to 0.1 for the standard method without any sub-iteration.

For a given $\Delta t$, the kinematic viscosity $\nu$ should be larger than $\Delta t U^2 / 4$, which indicates that an advection-diffusion equation with small kinematic viscosity is less stable.

When a simple underrelaxation is used during the sub-iteration, then the scheme can be written as follows:

$$\left[ \frac{1}{\Delta t} + \omega^2 \nu \right] \tilde{u}_k^{n+1} = -U i \omega \tilde{v}_{k-1}^{n+1} + \frac{\tilde{u}_k^n}{\Delta t},$$

(4.20)

$$\tilde{v}_k^{n+1} = (1 - \lambda) \tilde{u}_k^{n+1} + \lambda \tilde{v}_k^{n+1},$$

(4.21)

where $\lambda$ is between 0 and 1. The new sequence $\tilde{v}_k^{n+1}$ converges if $D_{sr} = \lambda^2 + (1 - \lambda)^2 \left( \frac{\omega U}{1/\Delta t + \omega^2 \nu} \right)^2 \leq 1$. This is satisfied if

$$\lambda > 1 - \frac{2}{1 + \left( \frac{\omega U}{1/\Delta t + \omega^2 \nu} \right)^2} = 1 - \frac{2}{1 + D_{su}^2}.$$  

(4.22)

Hence, if $D_{su} < 1$, then $\lambda$ can take any value between 0 and 1 and the sub-iteration is stable without relaxation. Suppose $D_{su} > 1$ then sub-iteration without relaxation is unstable because it violates the inequality equation (4.19). However, if $\lambda$ takes a value in the given range, then the sub-iteration with relaxation will converge and the scheme is unconditionally stable. Suppose $D_{su} \gg 1$, then $\lambda > 1 - \epsilon$ for stability and this is confirmed.
in previous numerical simulations summarized in Tables 4.2 and 4.3. In those tables, cases with increased parameter range of \( \lambda (0.0, 0.99) \) instead of \( (0.0, 0.9) \) show much more superior stability than cases with \( (0.0, 0.9) \).

4.4 Numerical simulations: unsteady Flow

Here, we report temporal accuracy of the schemes and comparison among sub-iteration, implicit scheme, and the standard method using time-dependent analytic solutions of the Navier-Stokes equations. Sub-iteration scheme is tested with unsteady flows past a cylinder, and pulsatile flows in straight and bend pipes and then compared with implicit scheme and the standard method.

4.4.1 Temporal accuracy of sub-iteration scheme

Here, we investigate the temporal accuracy of our new scheme using analytical solutions to the Navier-Stokes equations. The first analytic solution to the Navier-Stokes equations is given as

\[
\begin{align*}
  u(x, y, t) &= A \cos(\pi x) \cos(\pi y) \sin(t) \\
  v(x, y, t) &= A \sin(\pi x) \sin(\pi y) \sin(t) \\
  p(x, y, t) &= A \sin(\pi x) \sin(\pi y) \cos(t),
\end{align*}
\]

subject to the fluid body forces

\[
\begin{align*}
  f_x &= A \cos(\pi y) \cos(\pi x) \cos(t) - A^2 \pi \cos(\pi x) \sin(\pi x) \sin^2 t \\
    &\quad + \nu 2A \pi^2 \cos(\pi y) \cos(\pi x) \sin t + A \pi \sin(\pi y) \cos(\pi x) \cos(t) \\
  f_y &= A \sin(\pi y) \sin(\pi x) \cos(t) + A^2 \pi \cos(\pi y) \sin(\pi y) \sin^2 t \\
    &\quad + \nu 2A \pi^2 \sin(\pi y) \sin(\pi x) \sin t + A \pi \cos(\pi y) \sin(\pi x) \cos(t)
\end{align*}
\]

in [34]. This flow is periodic in time and space and simulated in a numerical domain \([0, 2] \times [-1, 1]\) with 2 quadrilateral elements and polynomial order 18 in each element as shown in Figure 4.9 (a). Dirichlet velocity boundary conditions are imposed on all sides and Neumann pressure boundary conditions are calculated from the previous velocity field.
Table 4.4 shows that the $L_2$ errors in velocity decay as $O(\Delta t^J)$, while the $L_2$ error in pressure decays as between $O(\Delta t^J)$ and $O(\Delta t^{J-1})$. Here, $J = 2, (3)$ corresponds to $J_i = J_p = J_e = 2, (3)$, respectively.

![Streamlines of time dependent flows](image)

Figure 4.9: Streamlines of time dependent flows in (a) equation (4.23) and (b) equation (4.26). The black straight lines and lines with arrows correspond to the element edges and streamlines, respectively.

Table 4.4: Errors in u-velocity of time dependent flow in equations (4.23). Final time $t = 1$, sub-iteration tolerance $= 10^{-6}$, and polynomial order $p = 18$.

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>$J = 2$</th>
<th>$J = 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$L_2$</td>
<td>$H_1$</td>
</tr>
<tr>
<td>0.1</td>
<td>6.940e-05</td>
<td>4.601e-04</td>
</tr>
<tr>
<td>0.01</td>
<td>6.236e-07</td>
<td>3.475e-06</td>
</tr>
<tr>
<td>0.001</td>
<td>6.353e-09</td>
<td>3.325e-08</td>
</tr>
</tbody>
</table>

The 2nd and 3rd order temporal accuracy is also confirmed with a time dependent flow with known exact solutions in [87]. This flow is also periodic in space and time, but the spatial period is different from the length of the domain causing more complicated boundary conditions than the previous example; e.g. the pressure at the boundary in the previous case,
i.e. equation (4.23), is zero for any time t. The exact solution \((u, v, p)\) is given as:

\[
\begin{align*}
u(x, y, t) &= \sqrt{3}\sin(\sqrt{2}x + t)\cos(\sqrt{3}y + t) \\
v(x, y, t) &= -\sqrt{2}\cos(\sqrt{2}x + t)\sin(\sqrt{3}y + t) \\
p(x, y, t) &= \sqrt{6}\sin(2x - \sqrt{5}y + 0.7t)\sin(\sqrt{5}y + 0.3t),
\end{align*}
\]

on the condition that the fluid body forces \((f_x, f_y)\) are assumed as:

\[
\begin{align*}
f_x &= \sqrt{3}\cos(\sqrt{2}x + \sqrt{3}y + 2t) + 3\sqrt{2}\sin(\sqrt{2}x + t)\cos(\sqrt{2}x + t) \\
&\quad + 2\sqrt{6}\cos(2x - \sqrt{5}y + 0.7t)\sin(\sqrt{5}y + 0.3t) \\
&\quad + 5\sqrt{3}\sin(\sqrt{2}x + t)\cos(\sqrt{3}y + t) \\
f_y &= -\sqrt{2}\cos(\sqrt{2}x + \sqrt{3}y + 2t) + \sqrt{3}\sin(2\sqrt{3}y + 2t) \\
&\quad + \sqrt{30}\sin(2x - 2\sqrt{5}y + 0.4t) - 5\sqrt{2}\cos(\sqrt{2}x + t)\sin(\sqrt{3}y + t).
\end{align*}
\]

This flow is simulated in a domain \([-1, 1] \times [-1, 1]\) with 4 quadrilateral elements and polynomial order 18 as shown in Figure 4.9 (b). Dirichlet velocity from the exact solution are specified on the boundary. Table 4.5 shows the 2nd and 3rd order accuracy with \(J = 2\) and \(J = 3\), respectively. At small \(\Delta t\), the errors of \(J = 3\) is smaller than those of \(J = 2\) by two order of magnitude.

Table 4.5: Errors in \(u\) velocity components of time dependent flow in equation (4.26). Final time \(t = 1\), sub-iteration tolerance = \(10^{-6}\), and polynomial order \(p = 18\).

<table>
<thead>
<tr>
<th>(\Delta t)</th>
<th>(J = 2) (L_2)</th>
<th>(J = 2) (H_1)</th>
<th>(J = 3) (L_2)</th>
<th>(J = 3) (H_1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>8.796e-04</td>
<td>3.341e-03</td>
<td>1.038e-04</td>
<td>4.127e-04</td>
</tr>
<tr>
<td>0.01</td>
<td>6.882e-06</td>
<td>2.655e-05</td>
<td>4.634e-08</td>
<td>5.283e-07</td>
</tr>
<tr>
<td>0.001</td>
<td>6.710e-08</td>
<td>2.598e-07</td>
<td>1.364e-10</td>
<td>1.985e-09</td>
</tr>
</tbody>
</table>

4.4.2 Sub-iteration versus fully-implicit scheme

In this section, we compare the stability and accuracy of three different schemes: implicit scheme, our sub-iteration scheme, and the standard scheme in \([76]\) with the first time dependent flow used in the previous section 4.4.1.
First, temporal accuracy of fully implicit scheme is confirmed using the exact solutions in equations (4.23) - (4.25). BDF of order \( J_i = 3 \) with \( J_e = 2 \) demonstrates 3rd order accuracy as in the standard method. BDF of order \( J_i = 2 \) with \( J_e \leq 2 \), or \( J_i = 3 \) with \( J_e = 1 \) achieves 2nd order temporal accuracy. For same integration order \( J_i \) and \( J_n \), higher \( J_e \) reduces error levels by factor of 2 or 3. At time step \( \Delta t = 0.001 \), \( L_2 \) errors in u velocity of \((J_i, J_e) = (2,1) \) and \( (2,2) \) are 5.27e-06 and 1.15e-08, respectively. In the same manner, \( L_2 \) errors in u velocity of \((J_i, J_e) = (3,1) \) and \( (3,2) \) are 4.35e-06 and 6.54e-09, respectively. However, \( J_e \geq 2 \) decrease the stability to the level of semi-implicit scheme.

For comparison among three schemes at \( J_i = 2 \), we measure errors and total CPU times for 100 time step at \( \Delta t = 0.01 \) which gives a CFL number around 1.4 ∼ 1.6. Among three cases - i.e. implicit, sub-iteration, and standard - sub-iteration scheme gives the best accuracy which is one order lower than the others as shown in Tables 4.6 and 4.7. We note that case ‘I2’ with \( J_e = 2 \) is more accurate than case ‘I1’ with \( J_e = 1 \) by two orders of magnitude. The standard scheme takes the least amount of time as expected. The CPU time for the sub-iteration scheme reduces dramatically from 174.50 second to 37.23 second by increasing the sub-iteration tolerance from \( 10^{-6} \) (case ‘T3’) to \( 10^{-2} \) (case ‘T1’). This raised tolerance leads to the error level increase by one order. However, such increased errors are still comparable or smaller than those of other methods. Moreover, we save computing time by 50 % with a large sub-iteration tolerance obtaining \( L_2 \) error in the order of \( O(10^{-6}) \).

4.4.3 Flow past a cylinder

The sub-iteration scheme is also tested with 2D flow past a cylinder which experiences periodic lift and drag forces due to the vortex shedding in the wake. Lift and drag coefficients are calculated and compared with coefficients using the standard method (See [7, 104, 78]). A cylinder of diameter 1 is located at the origin of a numerical domain, \([-5, 20] \times [-5, 5]\), with 675 quadrilateral elements and polynomial order 4. Flows at two Reynolds numbers, 100 and 500, are tested, which are based on the radius, and uniform and steady inlet velocity on the left side of the domain.

Our new scheme extends stable time step \( \Delta t \) up to 0.1 and and 0.05 at \( \text{Re} = 100 \) and 500, respectively while the standard scheme becomes unstable at \( \Delta t = 0.01 \) and \( \Delta t = 0.004 \). As the time step \( \Delta t \) increases, the number of iterations also increases. We note that the
Table 4.6: Errors in \((u,v)\) of implicit scheme, sub-iteration scheme, and standard scheme in time dependent flow in equations (4.23) - (4.25). Time step \(\Delta t = 0.01\), final time \(t = 1\) and polynomial order \(p = 18\). Cases T0, T1, T2, and T3 use sub-iteration tolerance \(0.05, 0.01, 10^{-4}\), and \(10^{-6}\), respectively. Cases I1 and I2 have the integration order \((J_i, J_e) = (2,1)\) and \((2,2)\), respectively. * CPU-times in parenthesis correspond to Conjugate Gradient solver.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>(L_2)</th>
<th>(H_1)</th>
<th>CPU-time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Implicit (I1)</td>
<td>(4.17e-04, 3.48e-04)</td>
<td>(3.32e-03, 2.26e-03)</td>
<td>75.97</td>
</tr>
<tr>
<td>Implicit (I2)</td>
<td>(6.35e-06, 4.67e-06)</td>
<td>(4.91e-05, 3.17e-05)</td>
<td>76.05</td>
</tr>
<tr>
<td>Sub-iteration (T0)</td>
<td>(1.32e-05, 1.08e-05)</td>
<td>(1.88e-04, 1.79e-04)</td>
<td>24.47 *(23.63)</td>
</tr>
<tr>
<td>Sub-iteration (T1)</td>
<td>(2.63e-06, 2.50e-06)</td>
<td>(6.57e-05, 6.65e-05)</td>
<td>37.23 *(29.32)</td>
</tr>
<tr>
<td>Sub-iteration (T2)</td>
<td>(6.23e-07, 4.54e-07)</td>
<td>(3.42e-06, 2.30e-06)</td>
<td>107.15 *(90.79)</td>
</tr>
<tr>
<td>Sub-iteration (T3)</td>
<td>(6.22e-07, 4.54e-07)</td>
<td>(3.35e-06, 2.21e-06)</td>
<td>174.50 *(157.01)</td>
</tr>
<tr>
<td>Without relaxation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sub-iteration 1</td>
<td>(1.31e-06, 1.27e-06)</td>
<td>(5.49e-05, 4.26e-05)</td>
<td>9.99</td>
</tr>
<tr>
<td>Sub-iteration 2</td>
<td>(6.93e-07, 5.97e-07)</td>
<td>(4.81e-06, 5.04e-06)</td>
<td>14.83</td>
</tr>
<tr>
<td>Sub-iteration 3</td>
<td>(6.31e-07, 4.79e-07)</td>
<td>(3.78e-06, 3.20e-06)</td>
<td>19.27</td>
</tr>
<tr>
<td>Sub-iteration 4</td>
<td>(6.23e-07, 4.59e-07)</td>
<td>(3.49e-06, 2.58e-06)</td>
<td>23.91</td>
</tr>
<tr>
<td>Sub-iteration 5</td>
<td>(6.22e-07, 4.55e-07)</td>
<td>(3.39e-06, 2.35e-06)</td>
<td>28.79</td>
</tr>
<tr>
<td>With relaxation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sub-iteration 1</td>
<td>(1.11e-02, 9.62e-03)</td>
<td>(5.87e-02, 4.55e-02)</td>
<td>9.86</td>
</tr>
<tr>
<td>Sub-iteration 2</td>
<td>(2.63e-04, 2.09e-04)</td>
<td>(2.11e-03, 1.38e-03)</td>
<td>14.51</td>
</tr>
<tr>
<td>Sub-iteration 3</td>
<td>(6.00e-05, 4.59e-05)</td>
<td>(5.85e-04, 4.50e-04)</td>
<td>19.36</td>
</tr>
<tr>
<td>Sub-iteration 4</td>
<td>(1.77e-05, 1.43e-05)</td>
<td>(2.36e-04, 2.20e-04)</td>
<td>24.02</td>
</tr>
<tr>
<td>Sub-iteration 5</td>
<td>(6.65e-06, 5.97e-06)</td>
<td>(1.26e-04, 1.26e-04)</td>
<td>28.74</td>
</tr>
<tr>
<td>Sub-iteration 6</td>
<td>(3.20e-06, 3.04e-06)</td>
<td>(7.75e-05, 7.85e-05)</td>
<td>33.75</td>
</tr>
<tr>
<td>Standard</td>
<td>(6.34e-06, 4.67e-06)</td>
<td>(4.90e-05, 3.17e-05)</td>
<td>4.45</td>
</tr>
</tbody>
</table>

Computing time per time step is not linearly proportional to the number of iterations. The computational cost per sub-iterations decreases as the sub-iteration continues, because conjugate gradient (CG) solver converges fast due to the better approximate solution as an initial condition. For example, case ‘C3’ in Table 4.8 at Re 100 requires the 35 iterations on average and the number of CG iteration decreases from \((189, 52, 52)\) for pressure, \(u\) velocity, and \(v\) velocity to \((138, 8, 8)\) during the first 32 sub-iterations. Without consideration of reduction in the sub-iteration cost, however, the slight speedup gain can be achieved, e.g. at time steps \(\Delta t = 0.01 \sim 0.025\) at Re = 500 using the sub-iteration scheme. Using large sub-iteration tolerances changes \(C_L\) and \(C_D\) insignificantly while the iteration numbers can
Table 4.7: Errors in (u,v) of implicit scheme, sub-iteration scheme, and standard scheme in time dependent flow in equations (4.23) - (4.25). Time step $\Delta t = 0.1$, final time $t = 1$ and polynomial order $p = 18$. Cases T0, T1, T2, and T3 use sub-iteration tolerance $0.05, 0.01, 10^{-4}$, and $10^{-6}$, respectively. Case I1 has the integration order $(J_i, J_e) = (2,1)$.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$L_2$</th>
<th>$H_1$</th>
<th>CPU-time(sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Implicit (I1)</td>
<td>(2.13e-02, 2.42e-02)</td>
<td>(1.48e-01, 1.40e-01)</td>
<td>8.02</td>
</tr>
<tr>
<td>Sub-iteration (T0)</td>
<td>(8.11e-05, 9.81e-05)</td>
<td>(8.04e-04, 7.61e-04)</td>
<td>6.89</td>
</tr>
<tr>
<td>Sub-iteration (T1)</td>
<td>(6.93e-05, 8.23e-05)</td>
<td>(4.59e-04, 4.15e-04)</td>
<td>9.76</td>
</tr>
<tr>
<td>Sub-iteration (T2)</td>
<td>(6.82e-05, 8.04e-05)</td>
<td>(4.18e-04, 3.77e-04)</td>
<td>17.43</td>
</tr>
<tr>
<td>Sub-iteration (T3)</td>
<td>(6.82e-05, 8.03e-05)</td>
<td>(4.60e-04, 3.77e-04)</td>
<td>17.57</td>
</tr>
<tr>
<td>Without relaxation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sub-iteration 1</td>
<td>(1.13e-03, 5.04e-04)</td>
<td>(5.50e-03, 4.17e-03)</td>
<td>1.31</td>
</tr>
<tr>
<td>Sub-iteration 2</td>
<td>(3.59e-04, 2.33e-04)</td>
<td>(2.31e-03, 2.07e-03)</td>
<td>1.73</td>
</tr>
<tr>
<td>Sub-iteration 3</td>
<td>(1.65e-04, 1.25e-04)</td>
<td>(1.34e-03, 1.32e-03)</td>
<td>2.15</td>
</tr>
<tr>
<td>Sub-iteration 4</td>
<td>(9.90e-05, 8.61e-05)</td>
<td>(8.37e-04, 8.67e-04)</td>
<td>2.60</td>
</tr>
<tr>
<td>Sub-iteration 5</td>
<td>(7.60e-05, 7.34e-05)</td>
<td>(5.75e-04, 5.93e-04)</td>
<td>3.05</td>
</tr>
<tr>
<td>Sub-iteration 6</td>
<td>(6.89e-05, 7.20e-05)</td>
<td>(4.60e-04, 4.57e-04)</td>
<td>3.48</td>
</tr>
<tr>
<td>With relaxation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sub-iteration 1</td>
<td>(9.55e-02, 1.27e-01)</td>
<td>(5.07e-01, 5.99e-01)</td>
<td>1.3</td>
</tr>
<tr>
<td>Sub-iteration 2</td>
<td>(1.35e-02, 1.51e-02)</td>
<td>(9.28e-02, 8.76e-02)</td>
<td>1.74</td>
</tr>
<tr>
<td>Sub-iteration 3</td>
<td>(4.89e-03, 5.29e-03)</td>
<td>(3.65e-02, 3.37e-02)</td>
<td>2.18</td>
</tr>
<tr>
<td>Sub-iteration 4</td>
<td>(2.31e-03, 2.39e-03)</td>
<td>(1.81e-02, 1.70e-02)</td>
<td>2.61</td>
</tr>
<tr>
<td>Sub-iteration 5</td>
<td>(1.20e-03, 1.24e-03)</td>
<td>(1.03e-02, 9.92e-03)</td>
<td>3.05</td>
</tr>
<tr>
<td>Sub-iteration 6</td>
<td>(6.72e-04, 7.07e-04)</td>
<td>(6.40e-03, 6.27e-03)</td>
<td>3.46</td>
</tr>
</tbody>
</table>

be reduced dramatically as in case ‘C10’.

The comparison of lift coefficients shows good agreement between the standard method and our sub-iteration scheme as listed in Table 4.8. Figure 4.10 shows the time traces of lift and drag coefficients and changes of iteration numbers in $\Delta t = 0.01 \sim 0.05$. We note that the iteration number is affected by the velocity fields and it increases near the zero-crossings of time traces of $C_L$.

4.4.4 Pulsatile flow

Pulsatile flows is common in bioflows and the exact solution of a pulsatile flow is available [148] when flow through a rigid pipe with constant diameter is assumed. We study two cases of pulsatile flow in this subsection: pulsatile flow in a straight pipe and in a U-bend.
Table 4.8: Simulation Cases at Re = 100 and Re = 500 with large time step $\Delta t$ and polynomial order $p = 4$. Sub-iteration tolerance is set to $10^{-4}$ except case ‘C9’ and ‘C10’ use $10^{-3}$ and $10^{-2}$. The drag and lift coefficients ($D/(1/2\rho U^2$ and $L/(1/2\rho U^2$) are Root Mean Square values.

<table>
<thead>
<tr>
<th>Cases</th>
<th>Re</th>
<th>$\Delta t$</th>
<th>$C_D$</th>
<th>$C_L$</th>
<th>sub-iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>standard</td>
<td>100</td>
<td>0.005</td>
<td>1.4914</td>
<td>0.2568</td>
<td></td>
</tr>
<tr>
<td>standard</td>
<td>100</td>
<td>0.01</td>
<td>unstable</td>
<td></td>
<td></td>
</tr>
<tr>
<td>iterative(C1)</td>
<td>100</td>
<td>0.01</td>
<td>1.4929</td>
<td>0.2588</td>
<td>6</td>
</tr>
<tr>
<td>iterative(C2)</td>
<td>100</td>
<td>0.05</td>
<td>1.4919</td>
<td>0.2577</td>
<td>11</td>
</tr>
<tr>
<td>iterative(C3)</td>
<td>100</td>
<td>0.1</td>
<td>1.4920</td>
<td>0.2576</td>
<td>35</td>
</tr>
<tr>
<td>standard</td>
<td>500</td>
<td>0.001</td>
<td>1.5412</td>
<td>0.8834</td>
<td></td>
</tr>
<tr>
<td>standard</td>
<td>500</td>
<td>0.004</td>
<td>unstable</td>
<td></td>
<td></td>
</tr>
<tr>
<td>iterative(C4)</td>
<td>500</td>
<td>0.001</td>
<td>1.5450</td>
<td>0.8860</td>
<td>5</td>
</tr>
<tr>
<td>iterative(C5)</td>
<td>500</td>
<td>0.005</td>
<td>1.5356</td>
<td>0.8748</td>
<td>7</td>
</tr>
<tr>
<td>iterative(C6)</td>
<td>500</td>
<td>0.01</td>
<td>1.5313</td>
<td>0.8668</td>
<td>8</td>
</tr>
<tr>
<td>iterative(C7)</td>
<td>500</td>
<td>0.025</td>
<td>1.5270</td>
<td>0.8577</td>
<td>38</td>
</tr>
<tr>
<td>iterative(C8)</td>
<td>500</td>
<td>0.05</td>
<td>1.5303</td>
<td>0.8579</td>
<td>98</td>
</tr>
<tr>
<td>iterative(C9)</td>
<td>500</td>
<td>0.05</td>
<td>1.5320</td>
<td>0.8545</td>
<td>80</td>
</tr>
<tr>
<td>iterative(C10)</td>
<td>500</td>
<td>0.05</td>
<td>1.5316</td>
<td>0.8572</td>
<td>53</td>
</tr>
</tbody>
</table>

The former case will demonstrate the temporal accuracy of our scheme and the latter the overall speedup gain in simulations of cardiovascular flows.

**Straight Pipe**

The radius and length of the pipe is 1 and 4, respectively. At the inlet the Womersley velocity profile is specified and at the outlet constant pressure condition is imposed. Simulations start from the exact solution at $t = 0$ up to final time $t = 1.0$ or 5.0 with sub-iteration tolerance is $10^{-6}$. Polynomial order for spatial discretization is 4 or 6 with 10,000 tetrahedral elements. Table 4.9 shows that our scheme is stable and accurate up to $\Delta t = 0.5$ while the standard method becomes unstable above $\Delta t = 0.01$. Here, 2nd order accuracy is not clearly seen because of the low spatial resolution. As the polynomial order is increased from 4 to 6, 2nd order temporal accuracy is observed from $\Delta t = 0.1$ to $\Delta t = 0.001$ as in Table 4.10.

For different time step $\Delta t = 0.5$, 0.3, and 0.25, volumetric flow rates (VFR) are computed for the entire cardiac cycle and relative errors are calculated. While the velocity errors are in the order of $10^{-4} \sim 10^{-6}$, time trace of VFR at the inlet and relative errors of flow rate
Figure 4.10: Iteration numbers at Re = 100 and 500. (top) shows iteration numbers for time step $\Delta t = 0.05, 0.1$ and the phase relation between the number of iterations and the lift coefficient at Re = 100. (bottom) shows iteration numbers for time step $\Delta t = 0.025, 0.01$ at Re = 500.

are shown in Figure 4.11. The differences in VFR are negligible among the cases ‘F1’, ‘F2’, and ‘F3’ in Table 4.9 and the relative errors in flow rate are less than 0.3 % as shown in Figure 4.11 (bottom).

We also test the stability of our scheme in a pulsatile flow for the entire cardiac cycle at large time steps $\Delta t$, which violate the CFL condition at the systolic peak. In such cases, the standard scheme becomes unstable and the time step $\Delta t$ is limited by the peak velocity at the systolic peak of the cardiac cycle. With the same straight pipe geometry, specific simulation parameters includes the nondimensional period of the cardiac cycle, 70, and the Womersley number, 2.22. The CG tolerance is set to $10^{-12}$ and the sub-iteration tolerance is set to $10^{-3}$ to reduce the number of sub-iteration. The average VFR and velocity are $40 ml/min$ and $0.21 m/sec$, respectively. The average Reynolds number is 110 based on the average velocity and the radius of the pipe. The total wall-clock time, maximum CFL number, and
Table 4.9: Errors in velocity of pulsatile flow at a straight pipe. Final time \( t = 5 \), sub-iteration tolerance = \( 10^{-8} \), and polynomial order 4. Additionally, cases ‘F1’, ‘F2’, and ‘F3’ are simulated for an entire cardiac cycle to measure the accuracy in pulsatile flow rate at the outlet as shown in Figure 4.11.

<table>
<thead>
<tr>
<th>Solver</th>
<th>( \Delta t )</th>
<th>( u - L_\infty )</th>
<th>( v - L_\infty )</th>
<th>( w - L_\infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>iterative</td>
<td>0.5</td>
<td>1.889e-04</td>
<td>1.900e-04</td>
<td>2.812e-04</td>
</tr>
<tr>
<td>iterative</td>
<td>0.3</td>
<td>2.158e-05</td>
<td>2.160e-05</td>
<td>6.239e-05</td>
</tr>
<tr>
<td>iterative</td>
<td>0.25</td>
<td>8.243e-06</td>
<td>8.244e-06</td>
<td>5.816e-05</td>
</tr>
<tr>
<td>iterative</td>
<td>0.2</td>
<td>5.336e-06</td>
<td>5.334e-06</td>
<td>3.069e-05</td>
</tr>
<tr>
<td>iterative</td>
<td>0.1</td>
<td>1.329e-06</td>
<td>1.328e-06</td>
<td>6.889e-06</td>
</tr>
<tr>
<td>iterative</td>
<td>0.01</td>
<td>2.131e-08</td>
<td>1.975e-08</td>
<td>4.614e-07</td>
</tr>
<tr>
<td>iterative</td>
<td>0.001</td>
<td>2.507e-08</td>
<td>2.456e-08</td>
<td>4.321e-07</td>
</tr>
<tr>
<td>standard</td>
<td>0.01</td>
<td>2.111e-08</td>
<td>1.947e-08</td>
<td>4.599e-07</td>
</tr>
<tr>
<td>standard</td>
<td>0.001</td>
<td>2.501e-08</td>
<td>2.451e-08</td>
<td>4.337e-07</td>
</tr>
</tbody>
</table>

Table 4.10: Errors in velocity of pulsatile flow at a straight pipe. Final Time \( t = 1 \), sub-iteration tolerance = \( 1e^{-8} \), and polynomial order 6.

<table>
<thead>
<tr>
<th>Solver</th>
<th>( \Delta t )</th>
<th>( u - L_\infty )</th>
<th>( v - L_\infty )</th>
<th>( w - L_\infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>iterative</td>
<td>0.1</td>
<td>4.812e-05</td>
<td>4.812e-05</td>
<td>1.343e-04</td>
</tr>
<tr>
<td>iterative</td>
<td>0.01</td>
<td>5.575e-07</td>
<td>5.588e-07</td>
<td>1.913e-06</td>
</tr>
<tr>
<td>iterative</td>
<td>0.001</td>
<td>6.637e-09</td>
<td>6.640e-09</td>
<td>2.479e-08</td>
</tr>
<tr>
<td>standard</td>
<td>0.01</td>
<td>4.617e-07</td>
<td>4.624e-07</td>
<td>1.586e-06</td>
</tr>
<tr>
<td>standard</td>
<td>0.001</td>
<td>5.320e-09</td>
<td>5.319e-09</td>
<td>1.737e-08</td>
</tr>
</tbody>
</table>

maximum errors are summarized and compared between the standard method and our new scheme. The maximum time step for the new scheme is 0.3 while the standard method becomes unstable above \( \Delta t = 0.01 \) for polynomial order \( p = 6 \) and \( J_i = J_e = J_p = 2 \). Due to the large sub-iteration tolerance and large time step \( \Delta t \), the total CPU time is reduced by 70% compared to the standard scheme at the cost of accuracy. \( L_2 \) errors in velocity increase from \( 10^{-8} \) to \( 10^{-4} \). In this simulation, we intend to demonstrate stability of our scheme at large CFL numbers 10.50 and reduction in computation time by 70% for a cardiac cycle as summarized in Table 4.11.

**Flow in an U-bend**

Since the Womersley flow in a straight rigid pipe has an analytic solution, temporal accuracy is tested in the previous subsection. However, the flow has zero nonlinear term. Hence,
Figure 4.11: VFR and relative errors of flow rate at the outlet of straight pipe with pulsatile input

Table 4.11: Stability comparison at a pulsatile flow in a straight pipe. CPU time (sec) is the wall-clock time for simulation of one cardiac cycle with polynomial order 6.

<table>
<thead>
<tr>
<th>Solver</th>
<th>$\Delta t$</th>
<th>CPU time (sec)</th>
<th>CFL</th>
<th>$u - L_\infty$</th>
<th>$v - L_\infty$</th>
<th>$w - L_\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>iterative</td>
<td>0.4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(unstable)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>iterative</td>
<td>0.3</td>
<td>4069.</td>
<td>10.50</td>
<td>7.737e-04</td>
<td>7.586e-04</td>
<td>5.555e-03</td>
</tr>
<tr>
<td></td>
<td>0.25</td>
<td>5378.</td>
<td>8.86</td>
<td>7.775e-04</td>
<td>7.704e-04</td>
<td>2.907e-03</td>
</tr>
<tr>
<td>standard</td>
<td>0.02</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(unstable)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>standard</td>
<td>0.01</td>
<td>12600.</td>
<td>0.35</td>
<td>1.053e-08</td>
<td>1.272e-08</td>
<td>4.249e-07</td>
</tr>
</tbody>
</table>

we test our scheme with a flow in an U-bend pipe with 10,000 tetrahedral elements whose geometry shown in Figure 4.12. The flow conditions are average velocity 0.264 (m/sec) with mean VFR 50 mL/min. The nondimensionalized period of the cardiac cycle is 132, and the average Reynolds number 139 based on the diameter of 2 and the mean velocity, while the Womersley number is 1.818. The polynomial order in each element is set to 4. Using temporal integration order $J = 2$, the standard scheme and sub-iteration scheme are tested for an entire cardiac cycle mainly to show the maximum time step $\Delta t$. These schemes become unstable near the systolic peak when the flow rate and velocity are highest. As listed in Table 4.12, simulation at CFL number 14.525 is stable and the maximum stable
time step $\Delta t$ increases by 37.5 times. However, the speedup gain based on the wall-clock time is 3.75. This may not be a fair comparison because we cannot obtain the same accuracy for all cases studied. The main idea here is to show how fast we can get reasonably accurate solutions. We compare three cases ‘S1’, ‘T1’, and ‘T2’ by plotting velocity time traces at history points near the U-shape bend as shown in Figure 4.12. Over the cardiac cycle, the differences among the three cases are not significant during the diastole. However, some discrepancies are more pronounced near the systolic peak resulting in up to 7% changes in velocity. The number of iterations are $2 \sim 5$ in all cases due to the large tolerance in the order of $10^{-3}$. One can use adaptive method to capture the systolic peak.

Table 4.12: Simulation cases of pulsatile flow in an $U$-shape bend at large time steps $\Delta t$ and sub-iteration tolerances. CPU time (sec) is the wall-clock time for simulation of one cardiac cycle and simulations are performed with polynomial order $p = 4$. Velocity time traces at history points in cases ‘S1’, ‘T1’, and ‘T2’ are compared in Figure 4.12.

<table>
<thead>
<tr>
<th>Solver</th>
<th>$\Delta t$</th>
<th>Tolerance</th>
<th>CPU time (sec)</th>
<th>CFL</th>
<th>iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>iterative</td>
<td>0.1</td>
<td>1e-3</td>
<td>(unstable)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>iterative (T2)</td>
<td>0.075</td>
<td>1e-2</td>
<td>2191</td>
<td>14.525</td>
<td>3</td>
</tr>
<tr>
<td>iterative</td>
<td>0.05</td>
<td>1e-2</td>
<td>2827</td>
<td>9.644</td>
<td>2</td>
</tr>
<tr>
<td>iterative (T1)</td>
<td>0.05</td>
<td>1e-3</td>
<td>3139</td>
<td>9.605</td>
<td>5</td>
</tr>
<tr>
<td>iterative</td>
<td>0.01</td>
<td>1e-3</td>
<td>8348</td>
<td>1.932</td>
<td>3</td>
</tr>
<tr>
<td>standard</td>
<td>0.004</td>
<td></td>
<td>(unstable)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>standard (S1)</td>
<td>0.002</td>
<td></td>
<td>9874</td>
<td>0.394</td>
<td></td>
</tr>
</tbody>
</table>

### 4.5 Conclusions

We developed a semi-implicit spectral/hp element method for the Navier-Stokes equations which updates the nonlinear term, $u \cdot \nabla u$, in the Navier-Stokes equation and enables more accurate pressure boundary condition through sub-iterations at each time step. Our eigenvalue analysis and numerical simulations confirmed that our proposed method is unconditionally stable in the steady Stokes flow. The proposed method is tested in steady Stokes problem and Navier-Stokes problem resulting in unconditional stability and conditional stability up to CFL number 1000. In unsteady Navier-Stokes flow, our scheme is stable at CFL number close to $5 \sim 14$. This scheme is tested in 2D flow past a cylinder and 3D pulsatile flows. Flow simulations in a straight pipe and an U-bend under the pulsatile flow condition demonstrates $3 \sim 3.75$ speedup gains.
Figure 4.12: Velocity distribution and time traces of volumetric flowrate (VFR) and velocity at points ‘Pt 1’, ‘Pt 2’, ‘Pt 3’, and ‘Pt 4’. (a) u velocity distribution on the planes parallel to $y = constant$. (b) v velocity distribution on the planes.
Chapter 5

Fluid-Structure Interaction

5.1 Introduction

Fluid-structure interaction (FSI) analysis is necessary in engineering and biomedical problems due to large deformations, e.g. heart valves. In FSI, there are two approaches: monolithic and partitioned. Partitioned solvers use separate codes for fluid subdomain and solid subdomain [97, 43] because each subdomain solver is optimized and modularity makes upgrade or implementation of a new scheme or new material type easier. For example, each solver can employ very efficient preconditioners; new material type or formulation may need to be implemented in the future. In those situations, it might take a long time to upgrade a monolithic solver [11, 10, 62] which solves both subdomains in a single code. However, monolithic schemes are advantageous from the stability point of view. Degroote et al. compared the performances of a partitioned quasi-Newton technique and a monolithic Newton algorithm [31]. They report that the ratio of the computing time is between 1/2 and 4 in relatively small problems although they projected that this ratio would change easily, depending on the size of problems. Further comparative studies were performed by Heil et al. [63].

Using the partitioned approach, Causin et al. showed that the instability in the coupling is due to the effect of added mass [19]. The added mass effect is significant when the density of solid is comparable to fluid density, making explicit (weak) coupling unconditionally unstable while strong coupling is conditionally stable. The number of sub-iteration increases as the density ratio is approaching 1 and the material stiffness is getting smaller. Fernandez et al. proposed a projection method as a strong coupling in the pressure correc-
tion scheme, one of splitting scheme of the Navier-Stokes equation solver [42]. Vierendeels et al. proposed a strong coupling through calculating the Jacobian from reduced order models [141]. Degroote et al. [32] showed that an error mode with a low spatial frequency destabilizes the fixed-point iteration. Aitken acceleration with a dynamic relaxation factor was introduced for stability by Mok et al. in [99, 82]. The aforementioned studies and their implementations are based on the linear finite element method. Here we focus on the high-order method, i.e. spectral element method for FSI problems.

The spectral element method has been used both in computational fluid mechanics and solid mechanics [77, 35, 139]. VIV simulations of translational but rigid cylinders have been performed using the spectral/hp element method [78, 104]. Compressible flow around an aerofoil with moving boundaries was simulated using high-order discontinuous Galerkin method [89]. In these studies, the density ratio of solid to fluid was large and there was no need of strong-coupling, because the added mass effect was not significant and instability was not an issue. In VIV studies, the mass ratio for stable simulations were limited to $3 \sim 4$.

Structural subdomains are described as simple 1D linear-mass-spring, tensioned beam, or plate equations. Hence, in this study, we focus on strong-coupling, low density ratio, and coupling with a 3D elastodynamic solver in complex geometries.

More specifically, we present implementation of and numerical studies with FSI based on the spectral/hp element method. High-order coupling through interfaces with structured or unstructured meshes is developed and tested in three cases; i) 2D VIV at $\text{Re} = 100$, ii) pulsatile flows in flexible tubes, iii) pulsatile flow in a patient-specific ICA with a narrow-neck aneurysm. We implement fictitious mass and damping which do not change system dynamics but help stabilize the interaction. We analyze the effect of fictitious mass and damping on stability.

Intracranial arteries are surrounded by tissues, bones, or the cerebrospinal fluid (CSF) which is under pulsating motion. Small arteries are tethered to the brain. In most FSI simulations, however, inlet and outlets are clamped and traction-free boundary condition is employed for outer walls. Such boundary conditions will cause erroneous large deformations and consequently numerical instability in FSI simulations of long and compliant vessels, because such motion is not allowed in the brain. Hence, we try to model the peripheral environment, which is an essential step of blood flow simulation in long and compliant patient-specific geometries. We demonstrate that this new boundary condition enhances
the stability and reduces the computational cost thanks to the effective increase of density
and stiffness of blood vessel.

This chapter is organized as follows. In section 5.2 we briefly describe the governing
equations of fluid and solid with boundary conditions and underlying assumptions. We
also present solvers and the coupling technique in use. In section 5.4 all results of VIV
simulations are presented followed by results of 3D tubes and of patient-specific aneurysm
in sections 5.5 and 5.6, respectively. A new boundary condition with spring supports is pro-
posed and tested in section 5.7 followed by effect of density change on the wall deformations
in section 5.8. We make concluding remarks in section 5.9.

5.2 Numerical methods

We describe the governing equations in fluid and solid subdomains. Solvers, coupling
method, and relaxation scheme for stabilization are explained.

5.2.1 Fluid Solver, NEKTAR

We assume that the fluid is incompressible and Newtonian and hence the flow is governed
by the incompressible Navier-Stokes equations. Suppose that fluid occupies the volume
\( \Omega(t) \) and the boundary \( \partial \Omega \) of the fluid subdomain is composed of a union of three different
boundaries, i.e. \( \partial \Omega = \partial \Omega_s \cup \partial \Omega_i \cup \partial \Omega_o \), where \( \partial \Omega_s \), \( \partial \Omega_i \), and \( \partial \Omega_o \) denote the interfacial
boundary, inlet boundary, and outlet boundary, respectively. In order to accommodate the
moving boundaries, we use the arbitrary Lagrangian-Eulerian (ALE) framework with the
Navier-Stokes equation written as

\[
\begin{align*}
\frac{\partial^* u}{\partial t} + (u - w) \cdot \nabla u &= - \nabla p + \frac{1}{Re} \nabla^2 u, \quad x \in \Omega(t) \\
\nabla \cdot u &= 0 \quad \text{in} \ \Omega(t) \\
\n\end{align*}
\]

where \( u \) is the velocity of the structure on the interfacial boundary. Hence, we note
that \( w = u \) recovers the Lagrangian description and \( w = 0 \), i.e. the static mesh frame,
recover the Eulerian description of fluid motion. No slip boundary condition means that $w(x,t)$ on the boundary is equal to the velocity of the structure at the interface, and the derivative, $\frac{\partial^*u}{\partial t}|_{\chi}$ in equation (5.1a), corresponds to material derivative of velocity at the moving mesh frame. At the interface between fluid subdomain and solid subdomain, Dirichlet and Neumann type boundary conditions are imposed for the velocity and pressure, respectively. Velocity at the inlet is problem-dependent and is given either as uniform flow in case of cylinder VIV simulations or pulsatile Womersley profile in case of blood flow simulations; in both cases, the outflow is assumed to be fully developed. The pressure at the outlets is set to constant or flow-rate dependent one using RC-type boundary condition [58].

These Navier-Stokes equations are solved with NEKTAR, which implements the spectral/hp element method and utilizes the Jacobi polynomial basis to represent the geometry, velocity and pressure. This solver employs a high-order splitting scheme and each time step consists of sub-iterations which continue until the $L_\infty$ norms of velocity and pressure difference between two subsequent sub-iteration steps become less than a given tolerance. Each sub-iteration solves seven linear system equations that arise from the splitting scheme and mesh velocity update. At the first splitting substep, it updates the solution treating the nonlinear convection term explicitly. Then, pressure is obtained by a Poisson equation using an updated intermediate velocity and Neumann pressure boundary conditions. At the third substep, the new velocity is obtained by solving three inhomogeneous Helmholtz equations. For more details, we refer to [77].

Here we briefly describe how the nonlinear term and pressure boundary conditions are used during the sub-iteration. In the semi-implicit scheme in [76], the nonlinear term is extrapolated in time and the pressure boundary condition is set accordingly to satisfy the compatibility condition of the pressure equation. In the strong coupling where sub-iteration is employed, the nonlinear term can be updated every sub-iteration. In the first sub-iteration, it is extrapolated as in the standard method. At the first sub-iteration, for given previous time step solutions $u^{n-q}$, $q = 0, ..., J_p - 1$ we solve equations (5.2a) and (5.2b) for $u^{n+1}_1$. $J_e$ and $J_i$ denote the order of explicit extrapolation in time for the nonlinear term and stiffly stable time integration order. The coefficients $\alpha_q$ and $\beta_q$ are given in [76]. In most simulations $J_e = J_i = 2$ are used resulting in the 2nd-order temporal accuracy in fluid.
\[
\hat{u} - \frac{\sum_{q=0}^{J_e-1} \alpha_q u^{n-q}}{\Delta t} = -\sum_{q=0}^{J_e-1} \beta_q [(u - w) \cdot \nabla u]^{n-q} - \nabla p_1^{n+1},
\]
(5.2a)

\[
\frac{\gamma u_1^{n+1} - \hat{u}}{\Delta t} = \nu \nabla^2 u_1^{n+1},
\]
(5.2b)

for the first sub-iteration with the following pressure boundary condition:

\[
\frac{\partial p_1^{n+1}}{\partial n} = - \left[ \frac{\partial u^n}{\partial t} + \nu \sum_{q=0}^{J_e-1} \beta_q [(\nabla \times \omega)^{n-q}] + \sum_{q=0}^{J_e-1} \beta_q [(u - w) \cdot \nabla u]^{n-q} \right] \cdot n.
\]
(5.3)

From the second sub-iteration, \( u_1^{n+1} \) and \( p_1^{n+1} \) are available as better approximates of \( u^{n+1} \) and \( p^{n+1} \). For \( k \geq 2 \),

\[
\hat{u} - \frac{\sum_{q=0}^{J_e-1} \alpha_q u^{n-q}}{\Delta t} = -[(u - w) \cdot \nabla u]^{n+1}_{k-1} - \nabla p_k^{n+1},
\]
(5.4a)

\[
\frac{\gamma u_k^{n+1} - \hat{u}}{\Delta t} = \nu \nabla^2 u_k^{n+1},
\]
(5.4b)

with the following pressure boundary condition:

\[
\frac{\partial p_k^{n+1}}{\partial n} = - \left[ \frac{\partial u_k^{n+1}}{\partial t} + \nu (\nabla \times \omega)^{n+1}_{k-1} + [(u - w) \cdot \nabla u]^{n+1}_{k-1} \right] \cdot n,
\]
(5.5)

where \( n \) and \( k \) correspond to the time level and the sub-iteration step, respectively. Sub-iteration stops and moves to the next time step level if both \( |u_k^{n+1} - u_k^{n+1}|_\infty \) and \( |p_k^{n+1} - p_k^{n+1}|_\infty \) are less than a tolerance, e.g. \( 10^{-6} \) or \( 10^{-7} \). However, using larger tolerances such as \( 10^{-4} \) or \( 10^{-5} \) may not affect the accuracy of the solution but reduce the number of sub-iteration. Computational cost is not proportional to the number of sub-iteration because the convergence rate of the Conjugate Gradient (CG) solver in each sub-iteration step varies among the sub-iteration step \( k \). After the first 2-3 steps, the number of CG iteration in the CG solver reduces gradually. One of benefits of the sub-iteration scheme is that the nonlinear term, \( (u - w) \cdot \nabla u \) is updated and more accurate pressure boundary condition is available. Numerical simulations confirmed that in the steady flow, time steps increase to \( O(1.0) \) resulting in the CourantFriedrichsLewy (CFL) number around 100, and in unsteady flows at Reynolds number 100 \( \Delta t = 0.05 \sim 0.1 \) and CFL number close to 5 is achieved.
For more details on the effect of sub-iteration and new updated boundary conditions on the stability and accuracy, we refer the reader to chapter 4.

The mesh velocity in the flow region is obtained by solving three Laplace equations for three components of velocity with Dirichlet boundary conditions on the fluid boundaries [66]. Specifically, the mesh velocity at the inlet and outlet boundaries are set to zero and the mesh velocity at the solid interface boundaries are set to the velocity obtained from the solid subdomain [89]. Since the solid velocity at the interface is changing every sub-iteration, the mesh velocity is also updated from:

\[ \Delta w^n_k = 0, \]  
\[ \Delta w^n_k = 0 \]

with boundary conditions, \( w^n_k = 0 \) for inlets and outlets and \( w^n_k = v^n_{k-1} \) at the interface and \( v^n_{k-1} \) is the interfacial velocity determined by the elastodynamics equations. Once the mesh velocity in the fluid subdomain is obtained by solving the Laplace equation with Dirichlet boundary conditions, the mesh position \( X \) is updated every time step after the sub-iteration converges through the following backward difference formula (BDF).

\[ \frac{X^{n+1} - \sum_{q=0}^{J_e-1} \alpha_q X^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q w^{n-q}, \]  
\[ \frac{X^{n+1} - \sum_{q=0}^{J_e-1} \alpha_q X^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q w^{n-q}, \]

where \( \alpha_q \) and \( \beta_q \) are coefficients for stiffly stable time integration schemes in [76].

When the velocity and pressure fields are available, the hydrodynamic stresses at the wall are calculated through

\[ t = \sigma \cdot n_f, \quad \sigma = -p I + \mu (\nabla u + \nabla u^T), \]  
\[ t = \sigma \cdot n_f, \quad \sigma = -p I + \mu (\nabla u + \nabla u^T), \]

where \( n_f \) is the normal vector at the boundary of fluid subdomain pointing outward. Stresses at the wall are calculated in the physical space, then are transformed to the modal space.

### 5.2.2 Solid Solver

Here we describe the equations of structural motion used in our simulations: linear mass-spring system and 3D elastodynamic system subject to hydrodynamic forces.
The equation of translational motion of a rigid cylinder

In 2D simulations of VIV, a cylinder is modeled as a mass-spring system with structural damping. The cylinder subject to hydrodynamic forces undergoes a translational motion of a rigid body in crossflow \((y)\) direction; inflow direction motion is not allowed. Such a rigid body motion can be described by a scalar 2nd-order differential equation:

\[
M \ddot{y}_{k+1}^{n+1} + C \dot{y}_{k+1}^{n+1} + K y_{k+1}^{n+1} = f_{k}^{n+1},
\]

(5.9)

where \(y_{k+1}^{n+1}\) is the \(y\)-direction displacement at time step \(n+1\) and sub-iteration step \(k+1\); \(M\), \(C\), and \(K\) are mass, damping, and spring constant, respectively. Sub-iteration is introduced to cope with the instability due to the explicit hydrodynamic force \((f_{k}^{n+1})\).

In addition, we include fictitious mass \((M_f)\) and structural damping \((C_f)\) to enhance the stability of coupling as follows:

\[
(M + M_f)\ddot{y}_{k+1}^{n+1} + (C + C_f)\dot{y}_{k+1}^{n+1} + K y_{k+1}^{n+1} = f_{k}^{n+1} + M_f \ddot{y}_{k}^{n+1} + C_f \dot{y}_{k}^{n+1},
\]

(5.10)

where \(C + C_f = 2(\zeta + \zeta_f)\omega_n (M + M_f)\); \(\omega_n^2 = K/M\); \(f_{k}^{n+1}\) is the external force, i.e. pressure and viscous force, at time step \(n+1\) and \(k^{th}\) sub-iteration step. When the sequence \(y_{k}^{n+1}\), \(k = 1, 2, 3, \ldots\) converges, \(\ddot{y}_{k+1}^{n+1} \approx \ddot{y}_{k}^{n+1}\) and \(\dot{y}_{k+1}^{n+1} \approx \dot{y}_{k}^{n+1}\). Consequently, the terms with \(M_f\) and \(C_f\) on both sides cancel out. Hence, either \(M_f\) or \(C_f\) do not change the system dynamics.

Adding an acceleration term to the structure equation was introduced in [26] and these terms at both sides of the equation disappear when the sub-iteration converges. We show that this term does not change the dynamics of the problem and improves the convergence of the sub-iteration. It is shown to stabilize the simulations even when the mass of the thin structure becomes small.

3D elastodynamics equation : StressNEKTAR

A 3D object initially occupying domain \(\Omega_0\) is deformed to a new configuration \(\Omega\) at time \(t\). Let \(\mathbf{X}\) and \(\mathbf{x}(\mathbf{X}, t)\) denote the coordinate in the undeformed configuration and the displace-
ment at the location $X$ and at time $t$. Then such deformation can be described as

$$\rho \frac{\partial^2 \mathbf{x}}{\partial t^2} = \nabla \cdot \mathbf{\tau} + \rho \mathbf{b}, \quad \mathbf{x} \in \Omega t = \mathbf{\tau} \cdot \mathbf{n}, \quad \mathbf{x} \in \partial \Omega_N. \quad (5.11)$$

The weak form of the momentum equation governing the deformation can be expressed as:

$$\int_{\Omega} \rho \frac{\partial^2 \mathbf{x}}{\partial t^2} \cdot \phi d\Omega = - \int_{\Omega} \mathbf{\tau} : \nabla \phi d\Omega + \int_{\partial \Omega_N} \mathbf{t} \cdot \phi dS + \int_{\Omega} \rho \mathbf{b} \cdot \phi d\Omega, \quad (5.12)$$

where $\mathbf{\tau}$, $\mathbf{b}$, $\mathbf{t}$, and $\rho$ are the stress tensor, external body force, external traction force, and structural mass density, respectively. $\mathbf{x}(\mathbf{X}, t)$ is the displacement to be solved for while $\phi$ is the test function.

Under the assumption that deformation is small and material is linear elastic, the stress tensor $\mathbf{\tau} = C \mathbf{\epsilon}$, where $C$ is the material matrix with two material constants, Young’s modulus ($E$) and Poisson constant ($\nu$) and $\mathbf{\epsilon} = 1/2(\nabla \mathbf{x} + \nabla \mathbf{x}^T)$, where $T$ indicates the transpose of a tensor or matrix. The constitutive equation can be written in indicial notation:

$$\tau_{ij} = C_{ijkl}\epsilon_{kl}$$

$$C_{ijkl} = \frac{E}{2(1 + \nu)} (\delta_{il}\delta_{jk} + \delta_{ik}\delta_{jl}) + \frac{E\nu}{(1 + \nu)(1 - 2\nu)} \delta_{ij}\delta_{kl}. \quad (5.13a)$$

The fourth-order tensor $C_{ijkl}$ can be written as 2D matrix using Voigt notation, which is convenient for programming.

$$C = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix} 1 - \nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1 - \nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1 - \nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 - 2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 - 2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 - 2\nu \end{bmatrix} \quad (5.14)$$

Moreover, $\Omega$ in (5.12) can be replaced by $\Omega_o$, the undeformed configuration.

A high-order spectral element method which solves equation (5.12) was developed by Dong and Yosibash; please refer to [36], which elaborates on the formulations, algorithmic implementation, and scalability tests. The implementation, StressNEKTAR, employs continuous Galerkin formulation, and the trial and test functions are Jacobi polynomials,
the same library our flow solver, NEKTAR, is based on. StressNEKTAR can deal with all commonly encountered 3D element types including hexahedrons, prisms, tetrahedrons and pyramids. The code is highly parallelized through domain decomposition and MPI. Its scalability is demonstrated over 2000 processors in [36]. In this study, either prism or hexahedron elements are used, and the interface is composed of triangular or quadrilateral faces of these elements. This code is modified to enable sub-iteration at each time step and MPI communication with the fluid subdomain.

Spatial discretization of the equation results in a linear system of ODE from which we want to obtain \( a^{n+1}, v^{n+1}, x^{n+1} \) at time level \( t_{n+1} = (n+1)\Delta t \) and sub-iteration level \( k+1 \),

\[
Ma^{n+1}_k + Cv^{n+1}_k + Kx^{n+1}_k = f^{n+1}_{k-1},
\]  
(5.15)

where \( f^{n+1}_{k-1} \) is the external force calculated at the previous sub-iteration step \( k - 1 \). Proportional damping matrix \( C = \alpha M + \beta K \) is employed for some simulations.

The way to describe \( a^{n+1} \) and \( v^{n+1} \) determines a numerical time integration scheme and dictates its accuracy in time and stability. Two different time discretizations are used in this study: (i) Newmark scheme and (ii) backward difference with three steps [33]. The Newmark scheme can be written as

\[
x^{n+1} = x^n + \Delta tv^n + \frac{\Delta t^2}{2} [(1 - 2\beta)a_n + 2\beta a_{n+1}],
\]  
(5.16a)

\[
v^{n+1} = v^n + \Delta t [(1 - \gamma)a^n + \gamma a^{n+1}].
\]  
(5.16b)

The accuracy depends on the parameters \((\gamma, \beta)\). For example, \((\gamma, \beta) = (0.5, 0.25)\) corresponds to the second-order Newmark scheme with constat-average-acceleration. \((\gamma, \beta) = (0.9, 0.49)\) degrades to first-order accuracy, but gives numerical damping which suppresses spurious transient oscillations.

A three-step backward difference for the acceleration and velocity are given as

\[
a^{n+1} \Delta t = \gamma v^{n+1} + \left( \frac{5}{2} - 3\gamma \right) v^n + (3\gamma - 4)v^{n-1} + \left( \frac{3}{2} - \gamma \right) v^{n-2},
\]  
(5.17a)

\[
v^{n+1} \Delta t = \beta x^{n+1} + \left( \frac{5}{2} - 3\beta \right) x^n + (3\beta - 4)x^{n-1} + \left( \frac{3}{2} - \beta \right) x^{n-2}.
\]  
(5.17b)

\((\gamma, \beta) = (3/2, 3/2), (11/6, 11/6)\) correspond to the second-oder and the third-order BDF
schemes, respectively. $\gamma$ and $\beta$ are not necessarily the same and can be decided in consideration of stability and dissipation. In this study, $(\gamma, \beta) = (10/6, 10/6)$ is used to confirm that it gives the 2nd order accuracy in time.

5.2.3 Solid solver: effect of fictitious mass and damping

We analyze the effect of fictitious mass and damping on the sub-iteration and stability of FSI. As in 2D cases, fictitious damping and density which do not disturb the dynamics of the system is implemented. In such cases, the above semi-discrete equation (5.15) is written as

$$(1 + \rho_f)M a_k^{n+1} + ((\alpha + \alpha_f)M + \beta K)v_k^{n+1} + Kx_k^{n+1} = f_{k-1}^{n+1} + \rho_f M a_{k-1}^{n+1} + \alpha_f M v_{k-1}^{n+1}. \quad (5.18)$$

For notational convenience, let us rewrite equations (5.17a)-(5.17b) as

$$a^{n+1} = A_1 v^{n+1} + B_1 v^n + C_1 v^{n-1} + D_1 v^{n-2}, \quad (5.19a)$$
$$v^{n+1} = A_2 x^{n+1} + B_2 x^n + C_2 x^{n-1} + D_2 x^{n-2}. \quad (5.19b)$$

We note that $A_{1,2}$ and other coefficients are $O(1/\Delta t)$. When equations (5.19a)-(5.19b) are substituted into equation (5.18),

$$[A_1 A_2 (1 + \rho_f)M + A_1 ((\alpha + \alpha_f)M + \beta K) + K] x_k^{n+1}$$
$$= (A_2 A_1 \rho_f M + A_1 \alpha_f M) x_k^{n+1}$$
$$+ f_{k-1}^{n+1}$$
$$- M [B_2 v^n + C_2 v^{n-1} + D_2 v^{n-2} + A_2 (B_1 x^n + C_1 x^{n-1} + D_1 x^{n-2})]$$
$$- (\alpha M + \beta K) [B_1 x^n + C_1 x^{n-1} + D_1 x^{n-2}] . \quad (5.20)$$

For simple notation, let $\tilde{K}$ and $\tilde{K}_f$ denote

$$\tilde{K} = A_1 A_2 M + A_1 \alpha M + A_1 \beta K + K,$$
$$\tilde{K}_f = A_1 A_2 \rho_f M + A_1 \alpha_f M, \quad (5.21)$$

respectively and let $R$ denote the terms which do not change over the sub-iteration, but
depend on the previous time step solutions as follows:

\[
\mathbf{R} = \mathbf{R}(\mathbf{x}^{n-2}, \mathbf{x}^{n-1}, \mathbf{x}^n, \mathbf{v}^{n-2}, \mathbf{v}^{n-1}, \mathbf{v}^n) = \\
- \mathbf{M} \left[ B_2 \mathbf{v}^n + C_2 \mathbf{v}^{n-1} + D_2 \mathbf{v}^{n-2} + A_2 (B_1 \mathbf{x}^n + C_1 \mathbf{x}^{n-1} + D_1 \mathbf{x}^{n-2}) \right] \\
- (\alpha \mathbf{M} + \beta \mathbf{K}) \left[ B_1 \mathbf{x}^n + C_1 \mathbf{x}^{n-1} + D_1 \mathbf{x}^{n-2} \right].
\] (5.22)

Then equation (5.20) can be written as

\[
\begin{bmatrix}
\mathbf{\tilde{K}} + \mathbf{\tilde{K}}_f
\end{bmatrix} \mathbf{x}_{k+1}^{n+1} = \mathbf{\tilde{K}}_f \mathbf{x}_{k-1}^{n+1} + \mathbf{f}_{k-1}^{n+1} + \mathbf{R}.
\] (5.23)

For simplicity of analysis, suppose that the external force \( \mathbf{f}_{k-1}^{n+1} \) is known a priori and independent of sub-iteration step \( k \), then \( \mathbf{f}_{k-1}^{n+1} \) is replaced by \( \mathbf{f}^{n+1} \). equation (5.23) is written as

\[
\begin{bmatrix}
\mathbf{\tilde{K}} + \mathbf{\tilde{K}}_f
\end{bmatrix} \mathbf{x}_{k+1}^{n+1} = \mathbf{\tilde{K}}_f \mathbf{x}_{k-1}^{n+1} + \mathbf{f}^{n+1} + \mathbf{R}.
\] (5.24)

Suppose that the limit of the sequences \( \mathbf{x}_{k+1}^{n+1} \rightarrow \mathbf{x}^{n+1} \) for \( k = 1, 2, 3, \ldots \) exists and let \( \mathbf{e}_{k+1}^{n+1} \) denote the error at time step \( n+1 \) and sub-iteration step \( k \), i.e. \( \mathbf{e}_{k+1}^{n+1} = \mathbf{x}_{k+1}^{n+1} - \mathbf{x}^{n+1} \), and then the error equation can be obtained from equation (5.24) as

\[
\begin{bmatrix}
\mathbf{\tilde{K}} + \mathbf{\tilde{K}}_f
\end{bmatrix} \mathbf{e}_{k+1}^{n+1} = \mathbf{\tilde{K}}_f \mathbf{e}_{k-1}^{n+1}.
\] (5.25)

Hence, heuristically the ratio \( D_r = \mathbf{\tilde{K}}_f / (\mathbf{\tilde{K}} + \mathbf{\tilde{K}}_f) \) determines the decay rate of the error. First observation would be the ratio, \( D_r \), is between 0 and 1, but if \( \mathbf{\tilde{K}}_f \) is dominant, \( D_r \) is close to 1 and errors decay slowly resulting in more sub-iterations.

\( \mathbf{\tilde{K}} \) and \( \mathbf{\tilde{K}}_f \) are matrices, then we can employ the generalized eigenvalues (\( \lambda \)) and eigen-modes (\( \mathbf{v} \)) of mass matrix \( \mathbf{M} \) and stiffness matrix \( \mathbf{K} \) of \( \mathbf{M} \mathbf{v}_j = \lambda_j \mathbf{K} \mathbf{v}_j \). The set of \( \mathbf{v}'s \) diagonalizes both matrices \( \mathbf{M} \) and \( \mathbf{K} \). Let \( \Phi = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n] \) denotes the matrix that consists of eigenmodes such that \( \Phi^T \mathbf{M} \Phi = \mathbf{I} \) and \( \Phi^T \mathbf{K} \Phi = \Lambda \), where the \( \mathbf{I} \) and \( \Lambda \) are the identity matrix and a diagonal matrix with the eigenvalues \( \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \) on the diagonal. Now, the error vector \( \mathbf{e}_{k+1}^{n+1} \) in equation (5.25) can be written as \( \Phi \mathbf{e}_{k+1}^{n+1} \) and multiplying \( \Phi^T \) to the both sides of equation (5.25) results in

\[
\Phi^T \begin{bmatrix}
\mathbf{\tilde{K}} + \mathbf{\tilde{K}}_f
\end{bmatrix} \Phi \mathbf{e}_{k+1}^{n+1} = \Phi^T \mathbf{\tilde{K}}_f \Phi \mathbf{e}_{k-1}^{n+1}.
\] (5.26)
Since $\hat{\mathbf{K}}, \hat{\mathbf{K}}_f$ are made up of $M$ and $K$, $\hat{\mathbf{K}}, \hat{\mathbf{K}}_f$ are diagonalized as follows:

\[
\mathbf{\Phi}^T \hat{\mathbf{K}} \mathbf{\Phi} = A_1 A_2 \mathbf{\Phi}^T \mathbf{M} \mathbf{\Phi} + A_1 \alpha \mathbf{\Phi}^T \mathbf{M} \mathbf{\Phi} + A_1 \beta \mathbf{\Phi}^T \mathbf{K} \mathbf{\Phi} + \mathbf{\Phi}^T \mathbf{K} \mathbf{\Phi}
\]

\[
= A_1 A_2 \mathbf{I} + A_1 \alpha \mathbf{I} + A_1 \beta \mathbf{A} + \mathbf{A}
\]

\[
\mathbf{\Phi}^T \hat{\mathbf{K}}_f \mathbf{\Phi} = A_1 A_2 \rho_f \mathbf{\Phi}^T \mathbf{M} \mathbf{\Phi} + A_1 \alpha_f \mathbf{\Phi}^T \mathbf{M} \mathbf{\Phi}
\]

\[
= \rho_f A_1 A_2 \mathbf{I} + A_1 \alpha_f \mathbf{I}.
\]

(5.27)

Now, equation (5.26) is written as in a component form \((A_1 A_2 \rho_f + A_1 \alpha_f + A_1 A_2 + A_1 \alpha + A_1 \beta \lambda_j + \lambda_j) \hat{e}^{n+1}_k[j] = (A_1 A_2 \rho_f + A_1 \alpha_f)[\hat{e}^{n+1}_k[j]],\) The \(j^{th}\) component of \(\hat{e}^{n+1}_k\) decreases at the ratio of

\[
(A_1 A_2 \rho_f + A_1 \alpha_f)/(A_1 A_2 \rho_f + A_1 \alpha_f + A_1 A_2 + A_1 \alpha + A_1 \beta \lambda_j + \lambda_j),
\]

(5.28)

which we denote by \(D_r\). We note that \(A_1 \times A_2\) are \(O(1/\Delta t^2)\) and large \(\rho_f\) may dominate the numerator and the denominator for small eigenvalues \(\lambda_j\) and small time step \(\Delta t\). In such cases, \(D_r\) in equation (5.28) is close to 1, and the error decays much slower than small \(\rho_f\) or large eigenvalue \(\lambda_j\). Hence, fictitious density, \(\rho_f\), can not be too large especially when \(\Delta t\) is small. Our analysis also explains the empirical evidence that small structural density and stiffness makes the interaction less stable.

5.2.4 Aitken relaxation

Sub-iteration is employed to deal with the instability caused by the explicit coupling of fluid force to the solid domain. At each sub-iteration step, under-relaxation is performed in both the fluid and solid solvers as its benefits are reported in \([15, 99]\). The relaxation parameter, \(\lambda\), is calculated at each sub-iteration through the following rule.

\[
\hat{\mathbf{v}}_{k+1}^{n+1} = \lambda_k \hat{\mathbf{v}}_k^{n+1} + (1 - \lambda_k) \mathbf{v}_k^{n+1}.
\]

(5.29)

Here, \(\lambda_k\) is updated through the following Aitken scheme:

\[
\lambda_{k+1} = \lambda_k + (\lambda_k - 1) \frac{(\mathbf{Q}_k - \mathbf{Q}_{k+1}) \cdot \mathbf{Q}_{k+1}}{\| \mathbf{Q}_k - \mathbf{Q}_{k+1} \|^2},
\]

(5.30)

where \(\mathbf{Q}_{k+1} = \hat{\mathbf{v}}_{k+1}^{n+1} - \mathbf{v}_{k+1}^{n+1}\) and \(\cdot\) denotes relaxed solutions and \(\mathbf{v}_{k+1}^{n+1}\) is the original numerical solution from the equations. The calculated \(\lambda_{k+1}\) is forced to be in a set \([\lambda_{min}, \lambda_{max}]\) by
setting a closet value.

### 5.2.5 Coupling

Fluid and solid are coupled through kinematic and dynamics boundary condition at the interface, i.e.,

\[
\mathbf{u}_f \cdot \mathbf{n}_f = -\mathbf{v}_s \cdot \mathbf{n}_s \quad (5.31a)
\]

\[
\sigma_f \cdot \mathbf{n}_f = -\sigma_s \cdot \mathbf{n}_s, \quad (5.31b)
\]

where the subscripts \(f\) and \(s\) indicate fluid and solid, respectively. \(\mathbf{n}_f\) and \(\mathbf{n}_s\) are normal vectors at the interface pointing outward. These velocity and traction vectors are stored as coefficients in the modal space and they are transferred as many modes as available between the two domains using MPI communication.

The coupling is done through the following steps.

Step 1 time step \(n\), \(t_{\text{new}} = t_{\text{old}} + \Delta t\).

Step 2 sub-iteration step \(k\).

Step 3 (Fluid) Calculate the external traction vector on the fluid/solid interface surface.

Step 4 (Solid) Solve the elastodynamic equations for the deformation \((\mathbf{x}_n^k)\) using \(\mathbf{f}_{k-1}^n\) if \(k > 0\).

Solve the elastodynamic equations for the deformation \((\mathbf{x}_n^k)\) using \(\mathbf{f}^{n-1}\) at the last sub-iteration step if \(k=0\).

Step 5 (Solid) Perform relaxation using equation (5.29) to obtain \(\ddot{x}_n^k = \lambda_{k-1} \ddot{x}_n^k + (1 - \lambda_k) \ddot{x}^{n+1}_{k+1}\).

Step 6 (Solid) Obtain the velocity and acceleration \((\mathbf{v}_k^n, \mathbf{a}_k^n)\) using equation (5.17a,5.17b) or (5.16a,5.16b).

Step 7 (Solid) Send the acceleration \((\mathbf{a}_k^n)\) and velocity \((\mathbf{v}_k^n)\) at the wall to the fluid solver, NEKTAR.

Step 8 (Fluid) Update the velocity boundary condition with \(\mathbf{v}_k^n\) from the solid subdomain.

Step 9 (Fluid) Update mesh velocity by solving equation (5.6).
Step 10 (Fluid) Update the pressure boundary condition using equation (5.3) or (5.5).

Step 11 (Fluid) Solve for pressure ($p^n_k$) using equation (5.2a) or (5.4a).

Step 12 (Fluid) Solve the velocity ($u^n_k$) using equation (5.2b or 5.4b).

Step 13 (Fluid) Perform Aitken relaxation using equation (5.29) to obtain $\tilde{u}^n_k$.

Step 14 (Fluid) Calculate the traction at the fluid-solid interface using $\tau = \sigma_f \cdot n_f = \{-pI + \nu(\nabla u + \nabla u^T)\} \cdot n_f$.

Step 15 (Fluid) Send the traction to the StressNEKTAR.

Step 16 (Fluid) Check convergence by $\Delta u = |\tilde{u}^n_k - \tilde{u}^{n-1}_k|_\infty$ and $\Delta p = |p^n_{k+1} - p^n_k|$.

Step 16 (Solid) Check convergence by $\Delta x = |\tilde{x}^n_k - \tilde{x}^{n-1}_k|_\infty$.

Step 17 (Fluid,Solid) If $\Delta v$, $\Delta p$, and $\Delta x$ are less than a sub-iteration tolerance,

(Fluid) Update mesh position using (5.7);

(Fluid) $u^n = \tilde{u}^n_k, p^n = \tilde{p}^n_k$;

(Solid) $x^n = \tilde{x}^n_k, \nu^n = \tilde{\nu}^n_k, a^n = \tilde{a}^n_k$;

go to Step 1 ($n = n+1$) for next time step.

Step 18 Go to Step 2 ($k = k+1$) for next sub-iteration.

5.3 Numerical studies without interaction

In this section, we test subdomain problems, i.e fluid only or solid only without interaction between them. More specifically, we confirm that ALE formulation in the fluid subdomain satisfies the geometric conservation law (GCL). We also confirm numerically that sub-iteration with or without fictitious mass and damping does not change the temporal accuracy of solid solver. For the accuracy and stability of standalone fluid solver, please refer to chapter 4.

5.3.1 ALE - Geometric conservation law

The ALE formulation was applied to the finite element formulation in [69], and the velocity of moving mesh can be arbitrary. However, as Thomas and Lombard and other researchers
pointed out [134, 112, 43], the mesh geometry and mesh velocity should satisfy the GCL. GCL states that the rate of change of control volume should be equal to the integration of velocity flux on the surface of the control volume as in equation (5.32).

$$\frac{d}{dt} \int_{\Omega(t)} dV - \int_{\partial \Omega(t)} \mathbf{w} \cdot \mathbf{n} dS = 0,$$  \hspace{1cm} (5.32)

where \( \Omega(t) \) is the control volume at time \( t \) and \( \mathbf{w} \) is the mesh velocity with \( \mathbf{n} \) unit normal vector on the surface boundary \( \partial \Omega(t) \) of the control volume. This can be written in differential form using the \( \nabla \cdot \mathbf{w} = \frac{1}{J} \frac{DJ}{Dt} \), where \( J \) is the Jacobian of mapping of the moving meshes.

In order to confirm this GCL, uniform flow is simulated with moving meshes. Temporal accuracy is also tested because moving internal nodes with fixed boundaries should not affect an intended temporal accuracy. Here, we perform rigorous tests which check the accuracy of numerical solution with two flow cases with known analytic solution. One is the steady Poiseuille flow and the other is time-dependent flow.

In a steady Poiseuille flow, the center vertex is moved with \( u = \omega \cos(\omega t) \) and \( v = -0.3 \times \omega \sin(\omega t) \). The accuracy of ALE in the sub-iteration scheme is measured at final time \( t = 2 \) with time step \( \Delta t = 0.001 \). The \( L_2 \) errors of \( u \) and \( v \) velocity components are in the order of \( 10^{-8} \) as shown in Figure 5.1.

For time-dependent flow, the errors are measured at final time \( t = 1.0 \) with time step \( \Delta t = 0.001 \). As shown in Figure 5.2, the vertex at the center is moving with mesh velocity. \( u = 0.5 \sin(2\pi t) \) and \( v = 0.5 \cos(2\pi t) \). Here sub-iteration schemes are used with maximum allowed sub-iterations 20 and sub-iteration tolerance 1e-3 and \( L_2 \) errors in \( u \) and \( v \) are summarized in Table 5.1. Temporal accuracy of 2nd-order is obtained when \( L_2 \) errors in \( u \) and \( v \) are checked with time-dependent flow as summarized in Table 5.2. Moving mesh is illustrated in Figure 5.2 with the time-dependent flow at different times. These tests of spatial and temporal accuracy in steady and unsteady flows demonstrate that our ALE formulation and implementation of high-order integration satisfies GCL.

### 5.3.2 Solid solver with fictitious mass and damping

Here we confirm our analysis of the effect of fictitious mass and damping on convergence in previous section 5.2.3. With the following body force to obtain the exact solution, temporal
Figure 5.1: Moving mesh test. The center node is forced to move. (top) contour plot of $u$ velocity component with deformed moving meshes. (middle) contour plot of $v$ velocity. (bottom) mesh velocity vectors.

Accuracy is checked with a hexahedral element $[-1, 1] \times [-1, 1] \times [-1, 1]$ of polynomial order 4, the convergence tolerance $1.0e-9$, and the final time 1.

$$u = (1 + x) \sin(\omega t), \ v = w = 0.0, \ f_x = -(1 + x)\rho\omega^2 \sin(\omega t), \ f_y = f_z = 0.0,$$

where $\omega = 2\pi$. Structural damping is not included but the fictitious mass and damping are confirmed not to disturb the dynamics when time step $\Delta t$ is not too small. Second-order temporal accuracy is observed in different cases of $\Delta t$, $\rho$, $E$, $\rho_f$, $\zeta_f$. In general, fictitious mass and damping does not affect the result except the cases in which fictitious mass is dominant as summarized in Table 5.3.

Cases ‘SZ1’, ‘SZ2’, and ‘SZ3’ show 2nd-order temporal accuracy of the solid solver even
Table 5.1: $L_2$ errors in $u$, $v$ when the vertex is in forced motion with different polynomial order and time step $\Delta t = 0.001$.

<table>
<thead>
<tr>
<th>order</th>
<th>$u$</th>
<th>$v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.3365e-06</td>
<td>8.7734e-07</td>
</tr>
<tr>
<td>12</td>
<td>8.1770e-07</td>
<td>8.2049e-07</td>
</tr>
<tr>
<td>18</td>
<td>5.6875e-07</td>
<td>3.6264e-07</td>
</tr>
</tbody>
</table>

Table 5.2: $L_2$ errors in $u$, $v$ for different time step $\Delta t$ with integration order $J = 2$ when the vertex is in forced motion with polynomial order $p = 12$.

<table>
<thead>
<tr>
<th>time step $\Delta t$</th>
<th>$u$-$L_2$</th>
<th>$v$-$L_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>7.9411e-05</td>
<td>7.9692e-05</td>
</tr>
<tr>
<td>0.001</td>
<td>8.1770e-07</td>
<td>8.2049e-07</td>
</tr>
<tr>
<td>0.0001</td>
<td>8.1383e-09</td>
<td>8.1721e-09</td>
</tr>
</tbody>
</table>

with fictitious damping $\zeta_f = 1$. Comparison of cases ‘SZ3’ and ‘SZ4’ demonstrates that the presence of fictitious damping $\zeta_f = 1.0$ does not change the accuracy at all. Comparison of cases ‘SM4’ and ‘SM5’ also shows that increasing fictitious damping $\zeta_f = 1.0$ by factor of 10 does not change the accuracy at all. Since the fictitious damping term is less dominant than the fictitious mass by factor of $O(1/\Delta t)$, $\zeta_f$ up to $1/\Delta t = 1000$ is expected not to change the convergence rate or accuracy. Comparison of cases ‘SM2’, and ‘SM3’ shows a tendency that as the ratio $\rho_f/\rho$ increase, the sub-iteration begin to lose accuracy. The errors in case ‘SK2’ with $\rho_f/\rho = 5 \geq 1$ are much larger than case ‘SK1’ with $\rho_f/\rho = 0$. This shows that from accuracy point of view, large fictitious mass compared to actual mass slow down convergence causing larger errors than small fictitious mass cases. Hence, it is safe to say that $\rho_f$ should be smaller than $2\rho$ and $\zeta_f$ be smaller than $O(1/\Delta t)$.

Cases ‘SK1’, ‘SK2’, and ‘SK3’ have Young’s modulus $E = 1e5$, which decreases the ratio $D_r$ in equation (5.28) unless the fictitious mass or damping is dominant. Heuristically, $D_r$ can be written as

$$D_r = \frac{\rho_f + \zeta_f \Delta t}{\rho + \rho_f + (\zeta + \zeta_f) \Delta t + E \Delta t^2}.$$  \hspace{1cm} (5.34)

Suppose $\Delta t$ is so small due to stability conditions in a subdomain that $E \Delta t^2 \ll \rho$. Then $D_r$ is close to 1 unless $\rho_f \ll \rho$. In order words, when $\Delta t$ is small, using large fictitious mass for stability purpose is not a good practice. $D_r$ ($L_2$ errors) of cases ‘SK1’, ‘SK2’, and ‘SK3’ are about 0 (5.6e-08), 5/6 (3.2e-04), and 5/100 (5.18e-08), respectively. This clearly shows
that the accuracy of solid solver with sub-iterations depends on $D_r$ which is a function of fictitious mass and damping.

### 5.4 Numerical simulations I: Vortex-induced vibrations

In this section, strongly-coupled FSI is tested with 2D VIV in a wide range of density ratio. The stabilizing effect of the fictitious mass and damping is also confirmed. VIV simulations in this section are performed in a domain $[-5, 20] \times [-5, 5]$ with a cylinder of radius 1 located at the origin. The cylinder is allowed to move along the crossflow direction and a uniform steady flow is imposed at the inlet boundary. Fully developed natural boundary condition is used at the outlet. Periodic boundary condition is imposed along the crossflow direction creating infinite series of cylinders in parallel. The density of cylinder varies from
Table 5.3: Temporal accuracy of solid solver with fictitious mass/damping. $L_2$ error at final time $t = 1.0$ with sub-iteration tolerance $10^{-9}$.

<table>
<thead>
<tr>
<th>Cases</th>
<th>$\Delta t$</th>
<th>$\rho$</th>
<th>$E$</th>
<th>$\rho_f$</th>
<th>$\zeta_f$</th>
<th>$u-L_2$</th>
<th>$v-L_2$</th>
<th>$w-L_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SZ1</td>
<td>0.01</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
<td>4.3764e-03</td>
<td>2.6087e-04</td>
<td>2.6088e-04</td>
</tr>
<tr>
<td>SZ2</td>
<td>0.001</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
<td>4.3577e-05</td>
<td>2.5616e-06</td>
<td>2.5612e-06</td>
</tr>
<tr>
<td>SZ3</td>
<td>0.0001</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
<td>4.6019e-07</td>
<td>1.4836e-07</td>
<td>1.4025e-07</td>
</tr>
<tr>
<td>SZ4</td>
<td>0.0001</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>4.6531e-07</td>
<td>1.4737e-07</td>
<td>1.4147e-07</td>
</tr>
<tr>
<td>SM1</td>
<td>0.01</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>4.3859e-03</td>
<td>2.6062e-04</td>
<td>2.6062e-04</td>
</tr>
<tr>
<td>SM2</td>
<td>0.001</td>
<td>1.0</td>
<td>1.0</td>
<td>0.5</td>
<td>0.0</td>
<td>4.8737e-05</td>
<td>1.8042e-06</td>
<td>1.8036e-06</td>
</tr>
<tr>
<td>SM3</td>
<td>0.001</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>5.7042e-05</td>
<td>3.6173e-06</td>
<td>3.6169e-06</td>
</tr>
<tr>
<td>SM4</td>
<td>0.001</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>5.6889e-05</td>
<td>3.6130e-06</td>
<td>3.6125e-06</td>
</tr>
<tr>
<td>SM5</td>
<td>0.001</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>10.0</td>
<td>5.7372e-05</td>
<td>3.6814e-06</td>
<td>3.6809e-06</td>
</tr>
<tr>
<td>SK1</td>
<td>0.001</td>
<td>1.0</td>
<td>1e5</td>
<td>0.0</td>
<td>0.0</td>
<td>5.6562e-08</td>
<td>5.7956e-09</td>
<td>5.7832e-09</td>
</tr>
<tr>
<td>SK2</td>
<td>0.001</td>
<td>1.0</td>
<td>1e5</td>
<td>5.0</td>
<td>5.0</td>
<td>3.2122e-04</td>
<td>3.2739e-05</td>
<td>3.2739e-05</td>
</tr>
<tr>
<td>SK3</td>
<td>0.001</td>
<td>100.0</td>
<td>1e5</td>
<td>5.0</td>
<td>5.0</td>
<td>5.1806e-08</td>
<td>4.6699e-08</td>
<td>4.6377e-08</td>
</tr>
</tbody>
</table>

1 to 4 depending on test cases. The motion of cylinder is described by equation (5.9). Fully developed flow field with a fixed cylinder is used as an initial condition in the beginning of simulations. The cylinder at the origin is held fixed in the beginning of simulations and released later. The natural frequency of attached springs along the crossflow direction is $2\pi \times 0.215$, which is close to the vortex shedding frequency of the corresponding stationary cylinder. Small structural damping is introduced in some simulations. Various fictitious mass and damping are also introduced for comparison purposes. In this section, $\rho$, $\rho_f$, $\zeta$, $\zeta_f$, $M_i$ and $\epsilon_i$ denote mass ratio of a cylinder to fluid, fictitious mass ratio, structural damping coefficient, fictitious damping coefficient, maximum allowed sub-iteration number, and sub-iteration tolerance, respectively.

5.4.1 Fictitious mass and fictitious damping

We confirm that fictitious mass and damping introduced for stability do not modify the system and consequently the VIV of a cylinder or flow past it. Here we compare the VIV amplitude of three cases (mass ratio $\rho=4$ and fictitious mass ratio $\rho_f=0$, 2, and 4) with the result of weak coupling. In this comparison test, a large density ratio $\rho = 4$ and a small time step $\Delta t = 0.001$ is chosen so that the VIV simulation of the weak coupling is stable, although strong coupling (sub-iteration with Aitken relaxation) allows a much larger time step $\Delta t$. The amplitude change is negligible and the number of sub-iteration is as small
Figure 5.3: VIV displacements and sub-iteration numbers for different fictitious (added) mass cases. Density ratio $\rho = 4$, $Re = 100$, $\rho_f = 0, 2, \text{and } 4$. $\zeta=0.0$, $\omega_n = 2\pi \times 0.215$, ramping = 0.1, tolerance $\epsilon_t = 10^{-4}$, Max sub-iteration $M_i=100$, $(\lambda_{\min}, \lambda_{\max}) = (-0.2, 0.6)$, $\Delta t = 0.001$

as 3-5 in all cases as shown in Figure 5.3. The effect of fictitious mass on the number of sub-iteration seems unnoticeable. However, in case of low density ratio $\rho = 1$ with a time step $\Delta t = 0.01$, vanishing fictitious mass makes significant difference in the number of sub-iteration. Figure 5.4 shows that the average number of sub-iteration reduces from 53 to 20, i.e. by more than 50 % when a ficticious mass, i.e. $\rho = 1.0$ and $\rho_f = 1.0$ is used.

Now, we introduce a fictitious damping into the system, and we confirm that this fictitious damping does not change the dynamics of a given system either. We also check any effect of this fictitious damping and structural damping on the sub-iteration. The test parameters are listed in Table 5.4 for the crossflow-free cylinder. Figure 5.5 (a) and (b) shows that small structural damping decreases the VIV amplitude as expected and the fictitious damping does not change the amplitude. Including such small structural damping or fictitious damping does not seem to affect the number of sub-iteration. The average number of sub-iterations is around 22 for all cases and four cases do not show any significant difference among them as the sub-iteration is plotted against time in Figure 5.5 (c) and (d).
Figure 5.4: Sub-iteration number versus time unit. \( \rho = 1, \rho_f = 0 \) or \(1, \) \( \Re = 100, \zeta = 0.01, \omega_n = 2\pi \times 0.215, \) Max sub-iteration \( M_i = 100, \) Sub-iteration tolerance \( = 10^{-5} (\lambda_{min}, \lambda_{max}) \) of relaxation are -0.1 and 0.6, respectively. \( \Delta t = 0.01. \) Average sub-iteration numbers are 20 and 53.

Table 5.4: Simulation Cases with structural and fictitious damping at \( \Re = 100. \) \( \Delta t = 0.01, \rho = 1.0, \rho_f = 1.0 \) and sub-iteration tolerance \( = 10^{-5} \) for all cases.

<table>
<thead>
<tr>
<th>Cases</th>
<th>( \zeta )</th>
<th>( \zeta_f )</th>
<th>( \lambda_{min} )</th>
<th>( \lambda_{max} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>0.00</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.6</td>
</tr>
<tr>
<td>F2</td>
<td>0.01</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.6</td>
</tr>
<tr>
<td>F3</td>
<td>0.00</td>
<td>0.1</td>
<td>-0.1</td>
<td>0.6</td>
</tr>
<tr>
<td>F4</td>
<td>0.01</td>
<td>0.1</td>
<td>-0.1</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Effect of fictitious mass and fictitious damping on number of sub-iteration**

We study more systematically the effect of fictitious mass and structural damping on the number of sub-iteration with cases listed in Table 5.5. With a cylinder that is crossflow free, the fictitious mass varies from 0 % to 200 % of the actual mass ratio of the cylinder. Also we include small structural damping \( \zeta = 0.01 \) for some cases (from case A1 to A4) for comparison purposes. The time step is fixed at 0.05 which is 50 times larger than one in simulations with higher mass ratio.

Cases A1 and Z1 which do not have fictitious mass have far more number of sub-iterations as shown in Figure 5.6 (top). The average number of sub-iterations are 40, 25, 23, and 23 for A1-A4, respectively. Higher fictitious mass ratio (50 %, 100% and 200 % of cylinder mass) reduces the number of sub-iteration by almost 50 % as shown in Figure 5.6 (top) regardless of the presence of structural damping. The difference in the number
Figure 5.5: VIV displacements and sub-iteration numbers in cases F1-F4 with or without fictitious damping and structural damping coefficients. (b) shows the zoom-in of the region indicated by the pink rectangle in (a). (d) also shows the zoom-in of the time interval indicated by the pink rectangle in (c). Sub-iteration tolerance = $10^{-5}$ with maximum sub-iteration 100.

of sub-iteration among these cases (A2, A3, A4, Z2, Z3, Z4) is not significant. Hence, the presence of structural damping or fictitious damping seems not to change the convergence at all as clearly shown in Figure 5.6 (bottom). This is because the fictitious damping term is smaller by a factor of $O(1/\Delta t) \approx 100$ than fictitious mass term in the convergence ratio equations (5.34) and (5.28).

### 5.4.2 Effect of large sub-iteration tolerance

Sub-iteration tolerance used so far is as small as $10^{-5} \sim 10^{-9}$. Here, we test how FSI solutions are sensitive to sub-iteration tolerance, i.e. larger sub-iteration tolerances reduce the sub-iteration number without changing the displacement of VIV simulations. To that end, tolerances as large as $10^{-2} \sim 10^{-5}$ are tested with the following simulation parameters: $\rho = 1.0$, $\rho_f = 1.0$, $\zeta = 0.01$, relaxation parameter $(\lambda_{min}, \lambda_{max}) = (0.0, 0.06)$, and $\Delta t = 0.01$. 
Table 5.5: Simulation Cases with fictitious mass and structural damping at Re 100. \( \rho = 1.0, \Delta t = 0.05 \), and sub-iteration tolerance = \( 10^{-5} \) for all cases.

<table>
<thead>
<tr>
<th>Cases</th>
<th>( \rho_f )</th>
<th>( \zeta )</th>
<th>( \zeta_f )</th>
<th>( \lambda_{min} )</th>
<th>( \lambda_{max} )</th>
<th>sub-iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>0.0</td>
<td>0.01</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>40</td>
</tr>
<tr>
<td>A2</td>
<td>0.5</td>
<td>0.01</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>25</td>
</tr>
<tr>
<td>A3</td>
<td>1.0</td>
<td>0.01</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>23</td>
</tr>
<tr>
<td>A4</td>
<td>2.0</td>
<td>0.01</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>23</td>
</tr>
<tr>
<td>B1</td>
<td>0.0</td>
<td>0.01</td>
<td>0.5</td>
<td>0.0</td>
<td>0.6</td>
<td>45</td>
</tr>
<tr>
<td>B2</td>
<td>0.5</td>
<td>0.01</td>
<td>0.5</td>
<td>0.0</td>
<td>0.6</td>
<td>25</td>
</tr>
<tr>
<td>B3</td>
<td>1.0</td>
<td>0.01</td>
<td>0.5</td>
<td>0.0</td>
<td>0.6</td>
<td>24</td>
</tr>
<tr>
<td>B4</td>
<td>2.0</td>
<td>0.01</td>
<td>0.5</td>
<td>0.0</td>
<td>0.6</td>
<td>24</td>
</tr>
<tr>
<td>Z1</td>
<td>0.0</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>40</td>
</tr>
<tr>
<td>Z2</td>
<td>0.5</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>24</td>
</tr>
<tr>
<td>Z3</td>
<td>1.0</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>23</td>
</tr>
<tr>
<td>Z4</td>
<td>2.0</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6</td>
<td>23</td>
</tr>
</tbody>
</table>

Four cases ‘TOL1’, ‘TOL2’, ‘TOL3’, and ‘TOL4’ have different sub-iteration tolerance \( 10^{-5} \), \( 10^{-4} \), \( 10^{-3} \), and \( 10^{-2} \), respectively. Sub-iterations up to 100 are allowed per each time step.

Figure 5.7 shows that the average sub-iterations reduce from 21 to 8 and 5 for tolerance \( 10^{-5} \), \( 10^{-4} \), and \( 10^{-2} \), respectively. The sub-iteration numbers reduces by 75 %, but the changes in displacement \( y/D \) are not noticeable. The details in the flow field are compared among the cases. More specifically, velocity time traces at history points in the wake are also compared as shown in Figure 5.8. History points in the near-wake are marked with dots in Figure 5.8 (top). Streamwise or crossflow direction velocities and u-v phase diagrams are plotted at six points in the wake behind the cylinder moving in the crossflow direction. Comparison at all six points shows good agreements among the different cases.

### 5.4.3 Effect of large time step \( \Delta t \)

Here we test stability and sensitivity of sub-iteration number to the range of relaxation parameter. More specifically we increase the time step \( \Delta t \) by 60 times and check stability and convergence of the sub-iteration. Large time step which is not restricted by stability condition is desirable although it should be small enough to give accurate solutions. Since FSI is computationally expensive, large time step \( \Delta t \) may reduce the computational cost significantly. Moreover, small time step \( \Delta t \) increase the ratio \( D_r \) in (5.28) and deteriorate convergence of sub-iteration. Hence, we report VIV simulations with large time steps and
Figure 5.6: Comparison of sub-iteration numbers in cases A1-A4, cases B1-B4 and cases Z1-Z4. Time traces of sub-iteration numbers in cases A1-Z4 listed in Table 5.5. (top left) Time trace of number of sub-iteration for a fixed structural damping $\zeta = 0.01$ as the fictitious mass increases from 0 % to 200 %. (top right) Time trace of number of sub-iteration for a fixed structural damping $\zeta = 0.0$ as the fictitious mass increases from 0 % to 200 %. (bottom left) Time trace of number of sub-iteration for a fictitious damping $\zeta_n = 0.5$ as the fictitious mass increases from 0 % to 200 %. (bottom right) Comparison of sub-iteration numbers between $\zeta = 0.0$ (Z4) and $\zeta = 0.01$ (A4,B4) when the fictitious mass $= 2$.

How range of relaxation parameter changes the sub-iteration number at each time step. Simulation parameters are listed in Table 5.6 and we increase the time step $\Delta t$ by factor of 10 to 60 from the largest time step at which VIV simulations via standard NEKTAR are stable.

The plots of VIV displacements and time traces of velocity at history points are shown in Figure 5.9. The VIV motions agree well among all cases ‘T1’, ‘T2’, and ‘T3’ as shown in Figure 5.9 (a). The time traces of fluid velocity at a history point also show good agreements among the cases as shown in Figure 5.9 (b) and (c).

The number of sub-iteration in case ‘T1’ does not change over the cycle. Cases ‘T2’ and ‘T3’ with time step $\Delta t = 0.05$ and 0.06, respectively, show periodic peaks around the zero crossing $y/D = 0$ of the displacement. The number of sub-iteration steps of case ‘T3’ is as large as 65 on average and more than 100 in peak as shown in Figure 5.9 (d). The average number of sub-iteration are 19, 27, and 65 for case ‘T1’, ‘T2’, and ‘T3’, respectively.
Figure 5.7: $\rho=1.0$, $\rho_f = 1.0$, $Re = 100$, $\Delta t = 0.01$, TOL1 = $10^{-5}$, TOL2 = $10^{-4}$, TOL3 = $10^{-3}$, ramp = 0.1 time unit, Max sub-iteration = 100, Upper/Lower limits = 0.6/0.0 of relaxation parameter, $\omega_n = 2\pi \times 0.215$, $\zeta = 0.01$. Averages = 21, 8, and 5 for TOL1, TOL2, and TOL3, respectively.

Table 5.6: Simulation parameters for large time step $\Delta t$ at Re = 100

<table>
<thead>
<tr>
<th>Cases</th>
<th>$\rho$</th>
<th>$\rho_f$</th>
<th>$\zeta$</th>
<th>$\zeta_f$</th>
<th>$\lambda_{min}$</th>
<th>$\lambda_{max}$</th>
<th>$\Delta t$</th>
<th>sub-iteration</th>
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<tr>
<td>T1</td>
<td>4.0</td>
<td>4.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.2</td>
<td>0.6</td>
<td>0.01</td>
<td>19</td>
</tr>
<tr>
<td>T2</td>
<td>4.0</td>
<td>4.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.2</td>
<td>0.6</td>
<td>0.05</td>
<td>27</td>
</tr>
<tr>
<td>T3</td>
<td>4.0</td>
<td>4.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.2</td>
<td>0.6</td>
<td>0.06</td>
<td>65</td>
</tr>
<tr>
<td>T4</td>
<td>4.0</td>
<td>4.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.2</td>
<td>0.8</td>
<td>0.06</td>
<td>20</td>
</tr>
</tbody>
</table>

In order to understand the large sub-iteration number of case ‘T3’ and to reduce it, if possible, convergence behavior of cases ‘T1’, ‘T2’, and ‘T3’ are compared at a time step when the error of case ‘T3’ does not reach the given sub-iteration tolerance within 100 sub-iterations. Figure 5.10 shows the changes in $\Delta V = |V_{k+1}^n - V_k^n|$, calculated relaxation parameters $\lambda$, adjusted relaxation parameters $\lambda_c$ over the sub-iteration. The relaxation parameter $\lambda$ is adjusted so that $\lambda_c$ is in the range ($\lambda_{min}$, $\lambda_{max}$). As the time step $\Delta t$ increases, $\Delta V$ decays very slowly and the Aitken acceleration suggests $\lambda$ around 0.8 for cases T2 and T3. However, due to the ($\lambda_{min}$, $\lambda_{max}$) of the relaxation parameter, the upper limit 0.6 is used instead. For case T1 with $\Delta t = 0.01$, it converges fast before the relaxation parameter goes beyond the limits and no chopping occurs. This suggests that increasing the range of the relaxation parameter for case T2 and T3. Hence in case T4, the upper
Figure 5.8: $\rho = 1.0$, $\rho_f = 1.0$, $Re = 100$, $\Delta t = 0.01$, $TOL1 = 10^{-5}$, $TOL2 = 10^{-4}$, $TOL3 = 10^{-3}$, $TOL4 = 10^{-2}$. mass ramp = 0.1 time unit, Max sub-iteration = 100, Upper/Lower limits = 0.6/0.0 of relaxation parameter, $\omega_n = 2\pi \times 0.215$, $\zeta = 0.01$.

limit is set to 0.8 and we compare convergence during sub-iteration between case T3 and T4 as shown in Figure 5.11. The instant is again chosen when case T3 does not converge within the maximum sub-iteration number 100 as indicated by the vertical lines in Figure 5.11 (a) and (b). We note that T4 converges as fast as case T2 with this new upper limit of relaxation parameter. Figure 5.11 clearly shows the effect of the cutoff limits of the relaxation parameter. This shows that the number of sub-iteration is sensitive to relaxation parameter, especially when the time step $\Delta t$ is large.

5.4.4 VIV at $Re = 500$

VIVs with crossflow direction free cylinder at $Re = 500$ are simulated and the effects of fictitious mass, structural damping and the range of relaxation parameters are studied. The same cylinder and configuration described in the beginning of this section is used except that Reynolds number 500. The simulation parameters are listed in Table 5.7. Cases
Figure 5.9: VIV displacement convergence and sub-iteration numbers over the sub-iteration in different $\Delta t$ of cases ‘T1’, ‘T2’, and ‘T3’. Mass ratio $\rho_4$, fictitious mass $\rho_f 4$. $\zeta=0.0$, ramping = 0.1, Tolerance = $10^{-4}$, Max sub-iteration $M_i 100$, $(\lambda_{min}, \lambda_{max}) = (-0.2, 0.6)$. (b) and (c) show the time history of $u$ velocity component at (1.52, 0.00) and (1.79, 0.40), respectively. These history points correspond to ‘d’ and ‘e’ behind the cylinder marked in Figure 5.8.

$ATn (n=1,2,3,4)$ include system structural damping while cases $ZTn (n=1,2,3,4)$ have zero damping. Cases $DLn (n=1,2,3,4)$ have the same configuration as corresponding $ATn$ except that $DLn$ has different upper/lower bounds of the relaxation parameter. Time step $\Delta t = 0.01$ and the Reynolds number, 500, is based on the incoming velocity, $U$, and the diameter of the cylinder. Sub-iteration numbers are in the order of 40 ~ 50 for most cases, much larger compared to the previous cases ($Re = 100$). The convergence tolerance $10^{-5}$ is chosen and the maximum sub-iteration is set to 100.

Figure 5.12 shows that the fictitious mass has a dramatic effect on the number of sub-iteration as we observed the similar effect in VIV simulations at $Re 100$. The presence of fictitious mass reduces the number of sub-iteration by 50 %. Cases $DL1$ and $AT1$ with zero fictitious mass have two times larger number of sub-iterations of other $DLn$ and $ATn$ cases with non-zero fictitious mass as shown in Figure 5.13 (top). Average sub-iteration numbers are 83, 48, 43, 40, and 61, 31, 29, 27 for $AT1$-$AT4$ and $DL1$-$DL4$, respectively. The structural damping does not change significantly as cases $AT1$ and $AT4$ are compared...
Figure 5.10: VIV displacements and sub-iteration numbers in different $\Delta t$ in cases T1, T2, and T3. $\rho=4$, $\rho_f=4$. $\zeta=0.0$, ramping = 0.1, sub-iteration tolerance = $10^{-4}$, Max sub-iteration 100, range of relaxation parameter $(\lambda_{min}, \lambda_{max}) = (-0.2, 0.6)$. The straight line in the middle shows $\lambda_{max}$.

with zero damping cases ZT1 and ZT4, respectively in Figure 5.12 (bottom). The effect of upper/lower bounds of the relaxation parameter on the number of sub-iteration is also observed. Figure 5.13 (bottom) show that cases DL1 (DL4) has about 70% of sub-iteration numbers of cases AT1 (AT4).
Figure 5.11: Changes in the convergence behavior with different relaxation parameter limits (Comparison between case T3 and T4). V and relaxation parameter λ over the sub-iteration at time 260.6 which is indicated by the vertical bar in (a) and (b). Mass ratio 4, Added Mass 4. ζ=0.0, ramping = 0.1, Tolerance = 10^{-4}, Max sub-iteration 100, (λ_{min}, λ_{max}) = (-0.2, 0.6 ) for case T3 and -0.2 and 0.8 for case T4. (a) time traces of displacement (b) sub-iteration numbers of case T3 (dashed line) and T4 (solid line) (c) Velocity difference over the sub-iteration (d) Calculated relaxation parameter λ over the sub-iteration (e) Relaxation parameter after imposing the cut-off range.

Table 5.7: Simulation cases with fictitious mass and damping or different relaxation parameter ranges, and time step Δt=0.01 at Re 500, where Re is based on the diameter and the incoming velocity.

<table>
<thead>
<tr>
<th>Cases</th>
<th>ρ</th>
<th>ρ_f</th>
<th>ζ</th>
<th>λ_{min}</th>
<th>λ_{max}</th>
<th>Sub-iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>AT1</td>
<td>1</td>
<td>0.0</td>
<td>0.01</td>
<td>0.0</td>
<td>0.6</td>
<td>83</td>
</tr>
<tr>
<td>AT2</td>
<td>1</td>
<td>0.5</td>
<td>0.01</td>
<td>0.0</td>
<td>0.6</td>
<td>48</td>
</tr>
<tr>
<td>AT3</td>
<td>1</td>
<td>1.0</td>
<td>0.01</td>
<td>0.0</td>
<td>0.6</td>
<td>43</td>
</tr>
<tr>
<td>AT4</td>
<td>1</td>
<td>2.0</td>
<td>0.01</td>
<td>0.0</td>
<td>0.6</td>
<td>40</td>
</tr>
<tr>
<td>ZT1</td>
<td>1</td>
<td>0.0</td>
<td>0.00</td>
<td>0.0</td>
<td>0.6</td>
<td>83</td>
</tr>
<tr>
<td>ZT2</td>
<td>1</td>
<td>0.5</td>
<td>0.00</td>
<td>0.0</td>
<td>0.6</td>
<td>49</td>
</tr>
<tr>
<td>ZT3</td>
<td>1</td>
<td>1.0</td>
<td>0.00</td>
<td>0.0</td>
<td>0.6</td>
<td>44</td>
</tr>
<tr>
<td>ZT4</td>
<td>1</td>
<td>2.0</td>
<td>0.00</td>
<td>0.0</td>
<td>0.6</td>
<td>40</td>
</tr>
<tr>
<td>DL1</td>
<td>1</td>
<td>0.0</td>
<td>0.01</td>
<td>-0.2</td>
<td>0.8</td>
<td>61</td>
</tr>
<tr>
<td>DL2</td>
<td>1</td>
<td>0.5</td>
<td>0.01</td>
<td>-0.2</td>
<td>0.8</td>
<td>31</td>
</tr>
<tr>
<td>DL3</td>
<td>1</td>
<td>1.0</td>
<td>0.01</td>
<td>-0.2</td>
<td>0.8</td>
<td>29</td>
</tr>
<tr>
<td>DL4</td>
<td>1</td>
<td>2.0</td>
<td>0.01</td>
<td>-0.2</td>
<td>0.8</td>
<td>28</td>
</tr>
</tbody>
</table>
Figure 5.12: Sub-iteration numbers in cases AT1-ZT4 in Table 5.7. (top left) Time trace of number of sub-iteration for a fixed structural damping $\zeta = 0.01$ as the fictitious mass increases from 0 % to 200 %. (top right) Time trace of number of sub-iteration for a fixed structural damping $\zeta = 0.0$ as the fictitious mass increases from 0 % to 200 %. (bottom left) Comparison of sub-iteration numbers between $\zeta = 0.0$ (ZT1) and $\zeta = 0.01$ (AT1), when the fictitious mass = 0.0 (bottom right) Comparison of sub-iteration numbers between $\zeta = 0.0$ (ZT4) and $\zeta = 0.01$ (AT4) when the fictitious mass = 2.0. Re = 500, $\Delta t = 0.01$, sub-iteration tolerance = $10^{-5}$, max sub-iteration = 100.

Figure 5.13: Sub-iteration numbers in cases AT1-AT4 and DL1-DL4 in Table 5.7. Re = 500, $\Delta t = 0.01$, sub-iteration tolerance = $10^{-5}$, max sub-iteration = 100.
5.5 Numerical simulations II: pulsatile flow in a pipe

In this section, we present FSI simulations of pulsatile 3D flow in flexible tubes. In contrast to previous section 5.4, the 3D elastodynamic equations are solved with StressNEKTAR which communicates with NEKTAR. In all cases, the tubes are assumed to have a density close to that of fluid. Solid subdomains are modeled as a linear elastic material, and simulations are performed in a wide range of physiologically reasonable Young’s modulus \( E \) and the Poisson ratio \( \nu \). More specifically, these material constants of flexible tube are from 1 to 30 MPa which covers the physiologically reasonable range of intracranial vessels of size 2-4 mm as tabulated in [2]. Tubes of radius \( R \) 1 mm and of length \( L \) 4 mm, 8 mm, 16 mm are tested with pulsatile flow of mean flow rate 20 ml/min. The thickness of the wall is 0.105 mm which is about 5.2 % of the diameter. \( \rho_f = 1060 \text{kg/m}^3 \) and \( \rho_s = 1.5 \times \rho_f \). The Young’s moduli of the vessel walls are set to \( E_1 = 0.29 \text{MPa} \) or \( E_2 = 1.48 \text{MPa} \) with the Poisson ratio 0.3-0.4. The Womersley velocity profile with 8 Fourier coefficients is imposed at the inlet boundary and fully developed flow, i.e. \( \partial u / \partial n = 0 \), at the outlet boundary. The mean velocity is 0.1060 m/sec. For pressure, constant pressure or flowrate dependent pressure, i.e. RC-type boundary condition, is set at the outlet. A full cardiac cycle is simulated for all three tubes with different length, and the displacement and velocity at history points are recorded.

5.5.1 Pulsatile Flow in a straight tube

Blood vessel wall motion under pulsatile flow is mimicked with pulsatile flow in a straight pipe, and results are compared with measurement data available in the literature. Here, \( L = 16 \text{mm} \) case is presented because the larger \( L/R \) is, the more stronger is the added mass effect and FSI is less stable due to the geometric effect. Figure 5.14 shows time traces of velocity and displacement at a history point located at the interface of tube of length 16 mm. Top figure shows that mesh velocity and structure velocity in the fluid domain is continuous at the interface as the continuity is imposed strongly through iteration. In the beginning of simulation, the structure shows transient oscillations which decay during the cardiac cycle due to the structural and fluid viscous damping. Here, the wall deformation near the inlet is larger than deformations near the outlet, because constant outlet pressure is set and the absolute pressure is transferred to the solid domain. In other cases that
Figure 5.14: (top) show the contour of $y$ direction mesh velocity in the fluid domain. (middle) shows the linearly decreasing pressure distribution and exaggerated wall deformation along the tube. (bottom) time traces of velocity and displacement of a point at the interface of solid and fluid domain indicated with a circle in the middle. Young’s modulus $E_2 = 1.48$ MPa.

follow, the pressure distribution is taken as a reference and then pressure changes from the reference is transferred so that the deformation along the tube is uniform as shown in Figure 5.15.

With a tube of length 4mm and of radius 1mm, wall displacements are compared among three cases, ‘M1’, ‘M2’, and ‘M3’. Cases ‘M1’ and ‘M3’ have the Young’s modulus $E = 0.29$ MPa while that of tube in case ‘M2’ is $E = 1.48$ MPa, 5 times stiffer than cases ‘M1’, and ‘M3’. The outlet boundary condition for case ‘M3’ is modified so that the absolute pressure is 10 times higher than those of case ‘M1’ and ‘M2’. The reason for such pressure increase is to mimic the pressure change of 40 mmHg from the diastole to the systolic peak. In RC-type boundary condition, increasing the downstream resistance will increase the pressure at the outlet. In all three cases, the differential pressure with respect to a reference pressure taken in the beginning of simulation is transferred to the solid subdomain and the displacement is
Figure 5.15: (top) Contour plots of u-displacement at four time instants marked with straight lines. (bottom) time traces at a history point (z = 2) of displacement, pressure, and velocity. The Young’s moduli of ‘M1’, ‘M2’, and ‘M3’ correspond to 0.29 MPa, 1.48 MPa, and 0.29 MPa, respectively. The outlet boundary condition of case ‘M3’ increases the pressure level 10 times (increasing the downstream resistance by 10 times).

more or less uniform along the tube although fluid pressure linearly decreases along the tube from the inlet to the outlet. Cases ‘M1’ and ‘M2’ show the effect of stiffness change on the displacement and velocity. When the stiffness of case ‘M2’ increases 5 times, the velocity and displacement increase about 2.36 times. Due to the pressure level change in case ‘M3’, displacements of case ‘M3’ increases almost 10 times compared to those of case ‘M1’. We note the axial direction displacement follows the pulsatile flow rate changes, although the magnitude is 10 times smaller than radial direction displacement. For case ‘M3’, pressure at the outlet is set to 10 times higher by increasing the downstream resistance by 10 times to observe more physiological radial motion of blood vessel walls. The displacements of case ‘M3’ are around 0.075 mm, 7.5 % radial changes, which is close to 5 ~ 10 % radial changes.
Figure 5.16: Case ‘M3’: Contour plot of y direction displacement (left) and time traces of VFR, fluid/solid velocity and wall displacement (right). ‘Pt 19’, ‘Pt 21’, ‘Pt 18’, and ‘Pt 16’ are on the interface between fluid domain and solid domain, while ‘Pt 7’, ‘Pt 9’, and ‘Pt 13’ are along the center axis of fluid domain. Young’s modulus is $E_1 = 0.29$ MPa and the thickness of wall is 0.1mm.

The axial fluid velocity at the tube center ranges from 0.15 m/sec (diastole) to 0.26 m/sec and the displacement of the wall is 0.07 mm at the systolic peak which is comparable to 0.2 mm, the displacement of the carotid artery in [130]. The dimensional wall velocity is 0.6 mm/sec which is comparable to 5 mm/sec in [130], which measures the wall motion of the carotid. Their measurements are larger because the carotid artery is about 2-3 times larger than the tube used here. As in the previous case, the transient motion of wall is also observed in the beginning of simulation as in ‘U Vel.’ plot of Figure 5.16. In this section, we demonstrate that pulsatile flow is simulated in a compliant tube over a full cardiac cycle and simulation is stable. Moreover, a simulation with physiologically correct range of
parameters shows displacements comparable to in-vivo measurements.

5.5.2 Effect of fictitious mass and fictitious damping on stability

Here, we check the effect of fictitious mass and damping on the stability. Tubes of length 4 mm with radius 1 mm are used. The density ratio of solid to fluid is 1.2. Simulation parameters are Young’s modulus $E=5\times10^4$, Poisson ratio 0.3, structural damping coefficients $(0.001,0.001)$, $\Delta t = 0.001$, and relaxation parameter $(0.0, 0.98)$. Constant (zero) pressure boundary condition is used at the outlet and Womersley flow with mean volumetric flow rate 20 ml/min is imposed at the inlet. The fictitious mass and damping are listed in Table 5.8. These parameters are chosen so that fluid-structure interaction becomes unstable due to the small density ratio and small Young’s modulus. Relaxation parameters can be adjusted to achieve FSI stability. However, they are not adjusted so that the stabilizing effect of fictitious mass and damping is demonstrated. In order to measure the stabilizing effect, we run simulations for 4 hours and the number of time steps is counted.

Introduction of either fictitious mass or damping stabilizes the FSI simulations, which would be unstable otherwise, as summarized in Table 5.8. As the analysis in section 5.2.3 shows, small fictitious mass and damping helps reduce the effect of force coupling. If they are too large, then convergence rate becomes close to 1 and the sub-iteration slows down. This positive and negative effect is demonstrated in numerical simulations. When the fictitious mass increases from 0 to 2.0, the simulation becomes stable and the total number of steps increases from 203 to 902 by a factor of 4.5. When the fictitious density is larger than 2.0, however, the number of sub-iteration per time step increases and the total number of time steps for 4 hours decreases from 902 to 777.

When the fictitious damping is smaller than $1/\Delta t$, it is less dominant than mass or fictitious mass term in equation (5.28). First, fictitious dampings are selected to be smaller than the reciprocal of $\Delta t$, i.e. 1000. Hence, as the fictitious damping increases from 50 to 500, the FSI simulations become stable and the total number of steps increases from 303 to 474. When the damping goes beyond 2000, the total number of steps decreases from 942 to 842. Fictitious damping is not as effective as fictitious mass, but it enhances stability as the analysis shows.

The number of sub-iterations at each time step $n$ is plotted in Figure 5.17. Case ‘$\rho_f/2$’ with $\rho_f = 2$ shows the number of sub-iteration at each time is around 40 while case with
Table 5.8: Simulation cases of straight pipe with fictitious mass and structural damping

<table>
<thead>
<tr>
<th>Cases</th>
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<th>$\zeta_f$</th>
<th>Total number of steps</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
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<tr>
<td>$\rho_f2$</td>
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<td>0.0</td>
<td>902</td>
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<tr>
<td>$\rho_f4$</td>
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<td>0.0</td>
<td>836</td>
</tr>
<tr>
<td>$\rho_f5$</td>
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<td>0.0</td>
<td>777</td>
</tr>
<tr>
<td>$\zeta_f1$</td>
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<td>50.0</td>
<td>303</td>
</tr>
<tr>
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</tr>
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<td>942</td>
</tr>
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<td>$\zeta_f7$</td>
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<td>4000.0</td>
<td>842</td>
</tr>
</tbody>
</table>

Larger fictitious mass has around 50. Fictitious damping cases have 50-100 sub-iterations which result in smaller total number of steps for 4 hours than fictitious mass cases.

5.6 Numerical simulations III: pulsatile flow in a patient-specific aneurysm

Flow-structure interaction of pulsatile flow in a patient specific aneurysm model with flexible aneurysm sac is simulated. This simulation is intended to demonstrate the capability of our spectral element method for FSI. This aneurysm is located in the carvenous segment of right ICA and the subject was treated with coil embolization. The entire geometry is illustrated in Figure 2.1 of chapter 2. The thickness of aneurysm wall is around 0.1mm with Young’s modulus $E = 3.2$ MPa and Poisson ratio ($\nu$) 0.3. Outlet pressure boundary is obtained through a RC-type boundary condition. The pulsatile flow composed of 8 Fourier modes is imposed at the inlet. Density ratio of aneurysm wall to the fluid is set to 1.5 with time step $\Delta t = 0.01$. Average flow rate is set to 150 mL/min. Figure 5.18 shows the time traces of displacement and velocity at the fluid-solid interface. We also tested a case with 10 times larger Young’s modulus which is not presented here. Since the material is modeled as linear elastic and the wall deformation is small, displacements are expected to decrease by 10 times. For example, $y$ direction deformation at ‘pt 4’ decreases from $5e-4$ to $5e-5$. 
and the $z$ direction velocity of the wall or fluid particle attached to the wall decreases from $2e^{-4}$ to $2e^{-5}$.

### 5.7 New boundary condition with spring supports

Since the intracranial arteries are attached to the brain, go through intracranial base skull, or are surrounded by other tissues, constant pressure boundary condition on the peripheral side of the walls may not be an appropriate model. Physically clamping both ends of patient geometries is far from being realistic. Moreover, simulations with physiologically reasonable flow rates may not be stable numerically and physically in such geometries with clamping boundary conditions at the inlets and outlets. In order to model more reasonable boundary conditions for the peripheral environment of blood vessel walls and to make the flow stable physically and numerically, we propose two alternatives: fixed patches and linear springs. The former mimics bones or organs and the latter soft tissues. Fixed patches are effective in stabilizing simulations in complex geometry. When the boundary faces of elements marked with red circles are constrained (clamped) as shown in Figure 5.19, simulations are stable. In those simulations, inlets and outlets are free except a few elements with fixed boundary faces. Less than 10 element faces are fixed in both cases. As our beam analysis shows, many
Figure 5.18: Contour plots of wall velocity at three time instants (a,b,c) marked with lines on the right bottom plot. Velocity on the wall of a narrow-necked aneurysm on the internal carotid artery. Young’s modulus $E = 0.1 \text{MPa}$

supports are not necessarily more effective than one support with high spring constants. Please refer to Appendix C for more details. Compared to fixed patches, linear springs attached to vertices of an element is less restrictive. Hence, we focus on spring supports more than fixed patches in this section.

As a first step, the effect of clamping or supporting a face of a boundary element on deformation and stress field on the solid domain is compared. Springs with spring constant $K = 1e7$ are attached at four vertexes of an rectangular face of a boundary element. In both cases, both ends of the tube is clamped. The flow rate, 20 ml/min, is used by imposing the Womersley velocity profile at the inlet. Constant pressure is set at the outlet. Both cases show unnoticeable differences in the contour plot of $x$ direction displacement and $\sigma_{yy}$ as shown in Figure 5.20.

Vertices along the circumferential direction at certain $z$ coordinates are supported with linear springs. We refer this configuration as a ring of attached springs. With a tube of length/radius ratio 4, thee rings are placed along the tube between both clamped ends with equi-distance among them. All 96 springs are attached; 32 springs per 1 ring are attached along the circumference at three $z$ coordinates as shown in Figure 5.21 bottom (a).

The spring constants are $1e7, 1e5, 500, 50$, respectively. Simulation parameters are den-
Figure 5.19: (left) contour plots of displacement. (top) and (bottom) show different views for the U-shape bend and a narrow-necked aneurysm. Red circles mark the faces of boundary elements which are clamped (fixed).

Density ratio of solid to fluid 1.2, fictitious mass 0.5, Young’s modulus $1e5$, fictitious damping 1.0, Poisson ratio 0.3, damping coefficients (0.001,0.001), $\Delta t = 0.001$, and relaxation parameter (0.0, 0.98). The snapshots are taken at $t = 0.4$, i.e. 4000th time step. Constant (zero) pressure boundary condition is used at the outlet. Figure 5.21 shows the displacement and stress $\sigma_{xx}$ for cases with three rings. Except for the smallest spring stiffness $K = 50$, the displacements around attached springs is almost 0 and strong discontinuities of stress are observed where springs are attached. Differences between $K = 1e5$ and $K = 1e7$ are negligible.

We also check the effect of rings of springs on FSI stability. To that end, we choose a case in which FSI is unstable due to small density ratio and small Young’s modulus. A pipe
of length 4 with radius 1 is used and the wall thickness of solid domain is 0.105. Fluid and solid subdomains are discretized with 1792 and 512 hexahedral elements. The solid domain has two layers, and polynomials of order 3 are used for approximation. Constant (zero) pressure boundary condition is used at the outlet. Simulations are performed for 4 hours using 104 CPUs (72 for fluid and 32 for solid subdomain). The density ratio of solid to fluid is 1.2 with Young’s modulus $5 \times 10^4$. No fictitious mass or damping is introduced except damping coefficients $(\alpha, \beta) = (0.001, 0.001)$. Small time step $\Delta t = 0.001$ with relaxation parameter $[\lambda_{\text{min}}, \lambda_{\text{max}}] = (0.0, 0.98)$ is used although the relaxation parameter could be adjusted for stability.

We increase the spring constants from 0 to $1 \times 10^2$, $1 \times 10^4$, and to $1 \times 10^6$ (Cases ‘K1’ - ‘K4’ in Table 5.9), respectively without any fictitious damping or fictitious mass to isolate the effect of attached springs. Ring of springs with spring constants $K_s = 1 \times 10^2$ does not contribute to stability but springs with larger spring constants stabilize FSI as in Table 5.9.

Since the small density ratio of solid to fluid suffers the ‘added mass’ effect, larger solid density clearly stabilizes FSI and performs more time steps with less sub-iterations as in cases, ‘C3’, ‘C4’, and ‘C5’. With the same small solid density as in cases ‘C1’ and ‘C2’, combination of fictitious mass and damping with support springs stabilizes and reduces the number of sub-iterations.

<table>
<thead>
<tr>
<th>Cases</th>
<th>$\rho$</th>
<th>$\rho_f$</th>
<th>$\zeta_f$</th>
<th>$E$</th>
<th>$K_s$</th>
<th>Steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>K1</td>
<td>1.2</td>
<td>0.0</td>
<td>0</td>
<td>$5 \times 10^4$</td>
<td>0</td>
<td>unstable</td>
</tr>
<tr>
<td>K2</td>
<td>1.2</td>
<td>0.0</td>
<td>0</td>
<td>$5 \times 10^4$</td>
<td>$1 \times 10^2$</td>
<td>unstable</td>
</tr>
<tr>
<td>K3</td>
<td>1.2</td>
<td>0.0</td>
<td>0</td>
<td>$5 \times 10^4$</td>
<td>$1 \times 10^4$</td>
<td>109</td>
</tr>
<tr>
<td>K4</td>
<td>1.2</td>
<td>0.0</td>
<td>0</td>
<td>$5 \times 10^4$</td>
<td>$1 \times 10^6$</td>
<td>117</td>
</tr>
<tr>
<td>C1</td>
<td>1.2</td>
<td>0.5</td>
<td>50</td>
<td>$5 \times 10^4$</td>
<td>$1 \times 10^3$</td>
<td>308</td>
</tr>
<tr>
<td>C2</td>
<td>1.2</td>
<td>2.0</td>
<td>500</td>
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<td>$1 \times 10^5$</td>
<td>458</td>
</tr>
<tr>
<td>C3</td>
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<td>$1 \times 10^5$</td>
<td>885</td>
</tr>
<tr>
<td>C4</td>
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<td>5.0</td>
<td>50</td>
<td>$5 \times 10^4$</td>
<td>$1 \times 10^3$</td>
<td>1337</td>
</tr>
<tr>
<td>C5</td>
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<td>0.0</td>
<td>0</td>
<td>$5 \times 10^4$</td>
<td>0</td>
<td>1264</td>
</tr>
</tbody>
</table>
5.8 Effect of density change on wall deformation

The effect of solid density on the displacement and stress field under the pulsatile condition is investigated. Tubes of length 4 mm are clamped on both ends. A pulsatile flow is specified at the inlet with volumetric flow rate 20 ml/min and heart rate 120 BPM. The Young’s modulus of the tube is 5e6 and the ratio of solid to fluid is set to 10, 100, 500, and 1000 for cases ‘M1’, ‘M2’, ‘M3’, and ‘M4’, respectively. Time traces of displacement and velocity are plotted for comparison among all 4 cases with contour plots of cases ‘M1’ and ‘M3’. Only case ‘M4’ with density ratio 1000 demonstrates large deviations while time traces of three other cases ‘M1’, ‘M2’, and ‘M3’ show good agreements.

Pulsatile flow used in the simulations consists of 8 Fourier components among which the mean mode (DC component) is the strongest as well as intracranial blood flow in-vivo. The fundamental mode has the cardiac frequency, 1-2 Hz (2 Hz in our simulations) which is much lower than natural frequencies of the tube of order of 100. Substantial increase in density lowers the natural frequency of the tube and increases the inertia effect. However, such density change may not affect the response of structure at all, as demonstrated through numerical simulations, because the excitation frequency of blood flow is much lower than the natural frequency of the blood vessel walls. If a longer tube is used, however, the density is expected to play more important role. For longer tubes, the eigenvalues of the structure get smaller and the natural frequency of the tube may get closer to excitation frequencies, i.e. the harmonic frequencies in the pulsatile flow. Moreover, when a patient-specific geometry is used, the flow may become unstable as will be explained in the following chapters. In such cases, the pressure fluctuation may have 30 ~ 100 Hz frequency components and then the dynamic effect can be much more stronger than laminar flow cases. However, since the blood vessel is enclosed by or tethered to surrounding bones or other tissues, it seems to be reasonable to assume that blood vessels are closer to short tubes with both ends supported rather than to long tubes with both ends clamped. The fundamental mode of the blood vessels has short distance between nodes and the natural frequency is high. Hence, using higher density ratio may not change the results unless blood flow is unstable; this needs further investigation and validation.
5.9 Conclusions

We developed a high-order spectral/hp element method for fluid-structure interaction. Two solvers, NEKTAR and StressNEKTAR for fluid and solid subdomains, respectively, are based on the same spectral/hp element method and the same Jacobi polynomials. The fluid solver, NEKTAR, is a scalable parallel code with arbitrary Lagrangian-Eulerian formulation and mesh update every time step. The solid solver, StressNEKTAR, solves a linear elastodynamic equation with traction boundary condition at the fluid interface. Both solvers have spectral elements spatially and second or third-order accuracy in time. Both solvers were modified for sub-iteration to deal with the instability caused by the explicit coupling of fluid force to the solid domain. Velocity and traction boundary conditions at the interface are transferred in modal space and up to the highest mode available both in structured and unstructured meshes. The code has been developed and tested in 2D VIV and pulsatile flows in tubular pipes. Adding fictitious mass term to the elastodynamic equation, which will disappear when the sub-iteration converges, reduces the number of sub-iteration by 50%. Fictitious mass and damping enhances FSI stability and analysis combined with numerical examples shows that fictitious damping should be less than 2 times actual density and $2/\Delta t$, respectively. New boundary conditions which mimic the peripheral boundary conditions around the blood vessels walls are proposed and its stabilizing effect is demonstrated. We also demonstrate the capability of flow structure interaction with a patient-specific aneurysmal flow.
Figure 5.20: (left) contour plots of $u$ displacement and stress $\sigma_{yy}$ of tube with one fixed element. (right) $u$ displacement and stress $\sigma_{yy}$ of tube with one element supported by linear springs. The Young’s modulus is $1e4$ and the density is $1.2 \text{ g/cm}^3$. 
Figure 5.21: Contour plots of displacement and stress (a) Spring constant $K = 1e7$ (b) $1e5$ (c) 500 (d) 50. (top) Contour plot of x direction displacement ($u$). (bottom) Contour plot of stress $\sigma_{xx}$. Arrows and circles in bottom (a) show where the springs are attached.

Figure 5.22: Sub-iteration numbers versus time step in simulations performed for 4 hours. All simulation cases include three rings of springs.
Figure 5.23: Time traces (left) of displacement and velocity at history points on the interface and contour plots (right) of displacement and stress $\sigma_{xx}$. ‘M1’, ‘M2’, ‘M3’, and ‘M4’ correspond to density ratio 10, 100, 500, and 1000 with respect to fluid density, respectively. The contour plots on the right show the $x$ direction displacement and $\sigma_{xx}$ on the wall of the tubes.
Chapter 6

Flow Instability in Aneurysms

6.1 Introduction

Image-based computational fluid dynamics (CFD) simulations have been used to correlate WSS, pressure and other indicators with the formation and growth of an aneurysm [119, 24, 20]. In particular, impingement zones and areas of high WSS have been correlated to aneurysm formation, growth in size, or rupture [22]. It has been argued that blebs, ‘blisters on the aneurysm wall’, form in high WSS regions where the flow impinges into aneurysms [23]. Some authors [75, 16] claim that aneurysms tend to grow at an area where the endothelial layer is subject to abnormally low WSS. Hence, the ability to identify these critical locations in aneurysms, i.e. abnormally high or low WSS regions and impingement locations, would have significant implications for treatment.

Flow impingement regions inside aneurysms are reported to have a particular pattern of WSS/pressure distribution. The apex of flow impingement area, i.e. the local region of flow stagnation, is characterized by low WSS and higher static pressure, and is surrounded by a band of higher WSS and WSS-gradient [131]. An experimental study of an impingement area [98] showed that destructive remodeling involving loss of smooth muscle cells occurs at the region of high WSS and WSS gradient where the flow accelerates. Also, a more sensitive response of endothelial cells to turbulent oscillatory shear rather than to laminar and steady shear has been demonstrated experimentally [93, 100, 98]. Therefore, it seems important to understand the dynamic oscillatory behavior of WSS vectors in the impingement (stagnation) locations. To this end, we investigate systematically the oscillatory behavior of WSS vectors inside the aneurysm and the flow instability due to the presence of an aneurysm at
the posterior communicating artery (PCoA) origin.

Intraoperative Doppler recording of [126] showed flow fluctuations in the aneurysms of six patients out of 12. Spectra calculated from the parent vessels recordings did not show peaks except from the base pulsatile flow while spectra of the data from the aneurysms displayed several small peaks between 5 and 20 Hz. [41] recorded bruits from the sacs of 10 out of 17 intracranial aneurysms during surgery. The murmurs from aneurysms reported by [123] were associated with the fluctuating flow [125]. [118] also reported sounds from saccular aneurysms in eight of 11 patients and later they measured sound from experimental aneurysms in the common carotid bifurcation of dogs [117]. [21] performed simulations to show that ruptured aneurysms tend to have unstable (changing direction of inflow jet) aneurysmal flow unlike unruptured cases, but no further details of unstable flow are provided. 

A lateral aneurysm seems to be geometrically analogous to a cavity in a channel - a prototype flow which has been studied extensively. For the simplest cavity geometries, a streamline departing from the surface on the upstream edge of a rectangular cavity reattaches at or near the downstream edge of the cavity as described by [9]. Self-sustained oscillations including the cavity flow were reviewed in [115]. Cavity flow and its stability was studied numerically by [50]. In aneurysms in cerebral arteries, due to the effects of complicated geometry, we expect to find distinct regions of inflow and outflow at the mouths of wide-necked aneurysms. Such pattern of inflow and outflow may create inflection (change of curvature) of the velocity profile, which is the classic Rayleigh condition for instability [37]. This, in fact, was first hypothesized by [88]. Hence, we expect the instability to develop, probably only transiently because of the pulsatile nature of the blood flow, manifesting itself through velocity fluctuations of a distinctly higher frequency than the cardiac pulse.

Stability of pulsatile flow has been studied experimentally and numerically [39, 103, 128, 14]. Experimental study of flow in a straight pipe by [39] showed that pulsatile flows become ‘turbulent’ during the deceleration phase of oscillation at Reynolds number around 2000. [128] performed a linear stability analysis for plane pulsatile Poiseuille flow showing that pulsation may trigger instabilities. [103] measured velocity in the aorta of dogs and reported transition to turbulence at the end of systole.

\footnote{In these simulations, about 200 time step per cardiac cycle were used. Hence, possible temporal fluctuations were suppressed (Juan R. Cebral, private communication).}
Table 6.1: Datasets for 3D patient-specific models. The units of image size and resolution are voxels and $10^{-3} \text{mm}^3$/voxel, respectively.

<table>
<thead>
<tr>
<th>Patient</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Wide-necked</td>
<td>Narrow-necked</td>
<td>Two in proximity</td>
<td></td>
</tr>
<tr>
<td>Parent</td>
<td>ICA</td>
<td>ICA/PCoA</td>
<td>ICA/PCoA</td>
<td></td>
</tr>
<tr>
<td></td>
<td>sharp turns</td>
<td>smooth turns</td>
<td>tortuous turns</td>
<td></td>
</tr>
<tr>
<td>Size</td>
<td>8x8x10</td>
<td>6x6x3</td>
<td>3x4x2.5, 4x4x3</td>
<td>$\text{mm}^3$</td>
</tr>
<tr>
<td>Image Size</td>
<td>512x512x312</td>
<td>512x512x396</td>
<td>512x512x470</td>
<td>voxels</td>
</tr>
<tr>
<td>Resolution</td>
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<td>3.38x3.38x3.38</td>
<td>3.73x3.73x6.25</td>
<td>$10^{-3} \text{mm}^3$/voxel</td>
</tr>
<tr>
<td>Data Source</td>
<td>CT</td>
<td>3D-Digital Sub.</td>
<td>CT</td>
<td></td>
</tr>
</tbody>
</table>

CFD simulations in the carotid stenosis [45, 85, 60] were performed and intermittent turbulence during the decelerating systole was reported. However, the current work seems to be the first numerical study to report flow instability in aneurysms. Specifically we consider patient-specific geometries showing the spectra of fluctuating velocity inside aneurysms as well as time traces of WSS vectors on the aneurysm walls under pulsatile flow with volumetric flow rate (VFR) 150 – 400 mL/min in the ICA. Through a series of simulations, we report that aneurysmal flows may become unstable during the deceleration phase. We also aim to understand the distribution of WSS and its directional changes in aneurysms during the instability period.

In the following, we first present details of the geometric models and the simulation parameters in section 6.2 and subsequently results of simulations in section 6.3. Flow instability in a large intracranial network and effect of compliant wall is presented in section 6.4 and 6.5. We discuss findings and limitations of this study in section 6.6 followed by conclusions in section 6.7.

6.2 Methods

In this chapter, we analyze three representative vessel geometries harboring aneurysms with different characteristics selected from many patients we considered. For this retrospective review, Institutional Review Board (IRB) approval was obtained. Specifically, aneurysms in the supraclinoid ICA segment were considered; side (lateral) aneurysms are the most common and hence terminal aneurysms were not considered. Based on patients treated
Table 6.2: Simulation parameters for the patients A, B, and C. The Reynolds number, Re, is based on the diameter of the inlet, mean velocity, and kinematic viscosity. The Womersley number, $\omega_n$, is based on the radius ($R$) of the inlet, pulsatile circular frequency ($\omega = 2\pi f$), and kinematic viscosity ($\nu$).

<table>
<thead>
<tr>
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<th>AX</th>
<th>AL</th>
<th>AH</th>
<th>BS</th>
<th>BL</th>
<th>BH</th>
<th>BX</th>
<th>CL</th>
<th>CH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Patient</td>
<td>A</td>
<td>A</td>
<td>A</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>C</td>
<td>C</td>
</tr>
<tr>
<td>VFR (mL/min)</td>
<td>150</td>
<td>200</td>
<td>250</td>
<td>200</td>
<td>300</td>
<td>350</td>
<td>400</td>
<td>150</td>
<td>200</td>
</tr>
<tr>
<td>mean $U$ (m/s)</td>
<td>0.189</td>
<td>0.252</td>
<td>0.316</td>
<td>0.190</td>
<td>0.285</td>
<td>0.333</td>
<td>0.381</td>
<td>0.167</td>
<td>0.223</td>
</tr>
<tr>
<td>mean Re</td>
<td>204</td>
<td>271</td>
<td>340</td>
<td>235</td>
<td>353</td>
<td>413</td>
<td>473</td>
<td>191</td>
<td>255</td>
</tr>
<tr>
<td>$\omega_n = R\sqrt{\frac{U}{\nu}}$</td>
<td>3.04</td>
<td>3.04</td>
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<td>3.49</td>
<td>3.49</td>
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<td>6</td>
<td>4</td>
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<td>6.8</td>
<td>6</td>
<td>6.8</td>
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</tbody>
</table>

endovascularly, [102] reported that approximately 40.5% are small aneurysms ($< 10$ mm max size) with small neck ($< 4$ mm), 28.7% are small with wide neck ($> 4$ mm), 17.4% are large ($> 10$ mm) and 6% giant ($> 25$ mm). In general, approximately 15-20% of patients will have multiple aneurysms. According to statistics, the examples chosen in this study are representative of three types of aneurysms occurring in the supraclinoid ICA: wide-necked, small-necked, and multiple aneurysms (see Figure 6.1).

The first (patient A) has a very wide-necked aneurysm, resembling a fusiform aneurysm, in the supraclinoid ICA. The second (Patient B) has the posterior communicating artery (PCoA) harboring a relatively narrow-necked aneurysm. The third (patient C) developed two wide-necked aneurysms in the supraclinoid ICA. One of them is located at the root of the PCoA and the other one is downstream within a short distance. The aneurysm of patient B and the upstream aneurysm of patient C have the PCoA branches coming out of the aneurysm wall. Hence, all chosen aneurysms are located between the ophthalmic triangle and the ICA bifurcation into the anterior cerebral artery (ACA) and the middle cerebral artery (MCA) and approximately at the level of the eyes, behind the eye and towards the middle of the head.

Images from computed tomography angiography (CTA) or three-dimensional digital subtraction angiography (3D-DSA) were anonymized to remove any patient-specific data, and then exported in a DICOM format. The image resolutions and more detailed information of these data are explained in Table 6.1. The vessel geometries were manually extracted using in-house Matlab R2006b (The Mathworks, Natick, MA) tools, which enable a user to
pick a contour of vessel wall on a 2D DICOM image or to obtain an isosurface in a 3D data set. The contour lines and the image intensity level for isosurfaces are decided on a trial and error basis with the consideration of maximum gradient of image intensity, $I(x_i, y_i)$ or $I(x_i, y_i, z_i)$. Unstructured surface and volume meshes were generated using Gridgen version 15.12 (Pointwise Inc, Fort Worth, TX), a mesh generation software. The faces of tetrahedral elements at the vessel walls are projected onto curved surfaces generated by an interpolation algorithm (SPHERIGON), which requires the position of the vertices and the corresponding normal vectors. For details of the algorithm, we refer the reader to [92].

Based on sensitivity tests of inlet boundary conditions [18, 101, 107, 4], the inlet boundary conditions are imposed on the upstream of the lacerum ICA segment, which is shown in Figure 6.1 (center), to reduce the effect of a simplified boundary condition. Accordingly, long parent feeding vessels, which are not extended pipes but patient-specific ICA segments, are included in the computational domain to guarantee the development of the proper secondary flow upstream of aneurysms located in the supraclinoid segment. Small vessels less than 1 mm were not included because their effects are negligible [20] and all outlets were assumed to be efferent. The vessel walls were assumed to be rigid due to prohibitive computational cost of compliant vessel walls. The effect of compliant walls on the instability is discussed in section 6.5.

The natural boundary condition $\frac{\partial u}{\partial n} = 0$ for velocity at outlets. Constant pressure has been used for the pressure boundary condition at the outlets, since the pressure measurement at the outlet vessels or the relation between the flow rate and pressure are not available in most cases. In cases with multiple outlets, however, constant pressure condition should be avoided because flow division is solely determined by the resistance of the downstream vessel segment in the computational domain. In this study, however, flow instability in aneurysms does not seem to be affected even by substantial flow rate changes in the downstream bifurcation. Hence, constant pressure boundary condition is employed in most simulations of this study. “RC boundary condition”, a variant of Windkessel model, is used for the outflow sensitivity test with patient B and C geometries. Specifically, the flow rates at the outlets such as MCA, ACA, and PCoA are changed from those in constant pressure condition. In this type of boundary condition, the pressure is related to the flow rates through the differential equation $P(t) + RC \frac{dP(t)}{dt} = Q(t)R$, where $P(t)$, $R$, $C$, $Q(t)$ are the pressure at the boundary, the resistance, the capacitance, and the flow rate, respectively.
For the pulse rate, 80 beats per minute (BPM) were used in all simulations. At the inlet boundary, the Womersley velocity profile, which is the exact solution of pulsatile flow in a straight rigid pipe for a given flow rate, was imposed at the extended inlet. The flow rates either in the upstream or the downstream branches are not available. Hence, the VFR profile $Q(t)$ at the inlet was taken from the measurements of [94], and then approximated with $a_0 + \sum \{a_k \cos(2\pi kt/T) + b_k \sin(2\pi kt/T)\}$, where $T$ is the period of the cardiac cycle. Fourier coefficients were used to calculate the Womersley profile during simulations. The constant mode $a_0$ represents the average VFR, and the pairs of $a_k$ and $b_k$ ($k = 1, ..., 7$) normalized by constant mode $a_0$ are $(-0.152001, 0.129013)$, $(-0.111619, -0.031435)$, $(0.043304 - 0.086106)$, $(0.028871, 0.028263)$, $(0.002098, 0.010177)$, $(-0.027237, 0.012160)$, and $(-0.000557, -0.026303)$. Patient-specific VFR may have higher frequency components, but including more terms showed negligible change in the flow rate profile because of their small magnitudes compared to the average VFR. The pulsatility index in the VFR profile, i.e. the ratio of peak VFR to average VFR, is around 1.435 in the lower side of the range $1.66 \pm 0.16$ reported by [47]. The mean flow rate into the ICA ranges from 150 mL/min to 350 mL/min, which is in a physiologically reasonable range [47]. [95] and [30] also reported that the averaged ICA VFR is 248.4 mL/min and $255 \pm 42$ mL/min, respectively.

With the Newtonian assumption of blood, the fluid motion is governed solely by the incompressible Navier-Stokes equations with the no-slip boundary condition on the fixed wall. The possible effect of non-Newtonian property of blood on the result is discussed in section 6.6. The incompressible Navier-Stokes equations were solved with the parallel code NEKTAR [77], which implements the spectral/hp element method. NEKTAR employs two different formulations: (i) the Galerkin projection, and (ii) the discontinuous Galerkin projection. The first one is similar to the standard finite element method (FEM) whereas the second one is similar to finite volume method (FVM). Correspondingly, a semi-orthogonal and fully-orthogonal Jacobi polynomial basis is used in the form of tensor products of order $p$. For $p = 1$ and $p = 0$ we recover the standard FEM and FVM, but the multi-resolution capability of NEKTAR allows us to resolve local flow features without changing the mesh but simply increasing the polynomial order $p$. A typical range for $p$ is 5-10 to balance accuracy and computational efficiency. In terms of the mesh discretization,
polymorphic elements consisting of hexahedra, tetrahedra, prisms and even pyramids can be employed. The time discretization is based on second- and third-order stiffly stable semi-implicit schemes. The high accuracy obtained with high spatial/temporal accuracy and a small time step, $\Delta t$, is very important in resolving flow instabilities. For more details of the method and implementation, we refer the reader to [77]. NEKTAR has been validated for many different bioflows, e.g. see [121]. For the simulations in the present study, NEKTAR with the Galerkin projection is employed. We used the second-order semi-implicit scheme and Jacobi polynomial basis of order $p = 4 \sim 8$ on tetrahedral meshes. The polynomial order is increased when the mean flow rate increases and especially when the flow instability appears in order to confirm that the flow instabilities are not due to under-resolution.

The specific numerical simulation parameters for all cases from case ‘AL’ to case ‘CH’ are listed in Table 6.2. VFR ranges from 150 mL/min to 400 mL/min. We performed three, four, and two simulations with different VFRs for patients A, B, and C, respectively. Simulations with a fixed time step $\Delta t = 0.001 \sim 0.0005$ require 145000 $\sim$ 289000 steps taking 15-20 hours per cardiac cycle on parallel supercomputers utilizing 512-768 CPUs. Variations among cases are ascribed to the fact that computing time largely depends on the number of elements and nondimensional period $TU/L$, where $U$, $T$, and $L$ are mean velocity, period, and characteristic length, respectively.

The data from the third cardiac cycle were used for further analysis. We confirmed that the flow field reaches a stationary state within the first two cardiac cycles by calculating $D_V = |V(t) - V(t - T)|_\infty / |V(t)|_\infty$ and $D_Q = |Q(t) - Q(t - T)|_\infty / |Q(t)|_\infty$, where $V$, $Q$, and $T$ are a component of velocity at a history point, VFR at an outlet, and period of the cardiac cycle, respectively; here $| \cdot |_\infty$ denotes the maximum value. From the second to the third cycle, $D_Q$ diminishes from $O(1)$ to $O(10^{-4})$ and $D_V$ from $O(1)$ to $O(10^{-4})$ computed at some points located at the ICA and both aneurysms of patient C. To quantify the WSS dynamic fluctuations in the aneurysms as well as in the parent vessels, we compute the oscillating shear index (OSI) which is defined as $1/2 (1 - \int f \tau dt / |\tau| dt )$, where we denote the WSS vector by $\vec{\tau}$; $\vec{\tau}$ is defined by $\mu (\nabla u + \nabla^T u) \cdot n$, where $\mu$ and $n$ are the dynamic viscosity and the inward normal vector at the blood vessel wall. The angle changes of WSS vectors on the vessel walls were also calculated, where the angle is defined as the amount of deviation from a reference vector. This reference vector at each point can be any unit vector on the tangent plane. However, in this study we chose a unit vector parallel to WSS vector at the
systolic peak. We also visualize the WSS vectors on local patches where OSI is high.

6.3 Results: instability in aneurysms

Our computations provide a very large set of results, and only a small subset is presented here which demonstrate flow instability and WSS fluctuations. In cases AH, BH, and CH listed in Table 6.2, the aneurysmal flow becomes unstable with velocity fluctuations in the frequency range 20-50 Hz. Specifically, the flow in patient C became unstable with strong fluctuations in both velocity and WSS above VFR = 150 mL/min. For patients A and B, the flow instability became pronounced at higher VFRs, i.e. 250 and 400 mL/min, respectively.

6.3.1 Velocity profiles with inflection points

The presence of inflectional velocity profiles in arteries and associated instability was first hypothesized by [88]. Here we document such velocity profiles in different patient-specific aneurysms. Specifically, complicated velocity profiles along the straight lines in aneurysms are observed and inflection points are found, which indicate the possibility of flow instability according to the Rayleigh’s inflection criterion [37]. Specifically, Figure 6.2 shows several streamlines and velocity profiles along the line A-B inside the aneurysm at the systolic peak; inflection points are present in the velocity profiles. For patient C, Figure 6.3 shows profiles of the centerline velocity along the three lines inside the upstream aneurysm at two instants, i.e. at the systolic peak and during the decelerating systole. These graphs also show several inflection points. Here, the velocity profiles at two different instants look similar except that the overall amplitude changes. However, we note that the velocity profile at line ‘K’ shows increased negative velocity near the fundus of the aneurysm at instant (d); see the negative regions in the black lines labeled ‘K’ in the subplots (c-1) and (d-1) of Figure 6.3. We also checked the corresponding profiles during the diastole and they are closely similar.

6.3.2 Velocity time traces

The flow instability develops during the deceleration phase resulting in high frequency fluctuations in velocity time traces. Hence, velocity and pressure were recorded at up to 40 points upstream and downstream of aneurysms as well as inside the aneurysms to see any manifestation of instability; we call these points ‘history points’ in this paper. From
velocity time traces, their spectra are calculated and presented. Some velocity-time traces are shown in Figure 6.4 from the simulations of cases AH and AX (VFR = 250 mL/min, 150 mL/min), where case AX does not show strong fluctuations seen in case AH.

Patient B exhibits a very stable flow until VFR increases from 200 up to 350 mL/min as shown in Figure 6.5. Flow at VFR = 400 mL/min, however, demonstrates strong fluctuations as seen in the other patients A and C. Figure 6.6 shows velocity fluctuations in case CL (VFR = 150 mL/min) of patient C. The fluctuation amplitude becomes large between the systolic peak and the dicrotic peak, and decays toward the end of diastole. Figure 6.6 also shows similar trends in terms of velocity fluctuations, which start from the decelerating diastole and subsequently the flow returns to a smooth pulsatile state. Velocity traces both in the upstream and the downstream aneurysm show fluctuations. The velocity at ‘Pt 1’ in the upstream aneurysm starts to fluctuate earlier than at ‘Pt 10’ in the downstream aneurysm.

The spectra at history points ‘Pt 14’ and ‘Pt 15’ are shown in Figure 6.7 (top) revealing some peaks at frequency $f/f_{heart}$ around 16-50. The spectrum of patient B decays fast in Figure 6.7 (middle) while the frequency components in the spectrum of patient C are strong up to $f/f_{heart} = 100$, usually a sign of a longer-developed structure in the velocity towards transition to a distinctly turbulent-like motion, but not yet truly turbulent. The changes in spectra over the VFR change is clearly shown in Figure 6.7 (bottom) with the cases AX, AL, and AH of patient A. As the VFR increases from 150 mL/min to 250 mL/min, the decay of spectra becomes slower and peaks become more pronounced.

A history point ‘Pt 1’ of patient C, which is located inside the upstream aneurysm, has strong peaks around $f/f_{heart} = 22$. The frequency range of the three cases AH, CL, and CH are in good agreement with the Doppler recordings of [126] as well as the fact that flow instabilities start during the deceleration phase and that the flow returns to smooth pulsatile state either at the end of the systolic deceleration phase or at the end of diastole.

6.3.3 Oscillatory WSS vectors

Here we describe the oscillatory behavior of WSS vectors and the spatial variation of WSS oscillations. We also report on the movement of the stagnation region inside the aneurysm. The direction changes of WSS vectors are compared with the WSS vectors at the systolic peak.
Due to the velocity fluctuations we reported in section 6.3.2, the WSS vectors on the aneurysm wall fluctuate as shown in Figures 6.8 and 6.9 for patients A and B, respectively. Time traces of the magnitude and the direction of the WSS vectors at regions ‘L’, ‘M’, and ‘N’ on the aneurysm wall of patient A are plotted in Figure 6.8. The regions ‘L’ and ‘M’ have high OSI, while the region ‘N’ has low OSI close to 0. The WSS vectors in high OSI regions, i.e. ‘L’ and ‘M’, show direction changes over 180 degrees with large variation between two points at each region. In region ‘N’, however, the WSS vectors show similar fluctuations during the deceleration systole but with much smaller fluctuation amplitudes. Also, traces in region ‘N’ behave much more uniformly than regions ‘L’ and ‘M’ as shown in Figure 6.8. In the bottom two rows of Figure 6.8, WSS time traces of case AX at VFR 150 mL/min are shown for comparison of WSS between stable flow and unstable flow. Since the magnitudes are significantly different, it is hard to compare them directly. However, the WSS at higher VFR seem to be the scaled WSS of lower VFR superimposed with high frequency fluctuations.

We plot the time traces of the magnitude and direction of WSS vector at the red points marked in Figure 6.9 (left). The solid yellow lines indicate the locations of converging or diverging stagnation lines at the shown WSS vector field. Hence, Figure 6.9 (left) shows that the direction change of vectors along the solid yellow lines is minimal but transverse to these lines is maximal. More strikingly, visualizations at different times reveal that these lines are oscillating in space. The dotted yellow lines mark the boundaries of the spatial movement of the solid yellow lines over the cardiac cycle. Hence, the WSS vectors near these stagnation lines are experiencing significant oscillation over the cardiac cycle as their time traces plotted in Figure 6.9 (right) indicate. More specifically, the WSS vectors at points ‘L’ and ‘M’ show oscillations in both direction and magnitude. The reason for a smaller angle deviation near the systolic peak is that the angle changes of WSS vectors are computed with respect to the corresponding WSS vectors at the systolic peak. The WSS magnitude, however, shows larger oscillation magnitude at the systolic peak and decelerating systole similar to the velocity fluctuations. During the diastole, the WSS vectors change direction from 0 degree to ± 180 degrees while the magnitude does not change.

However, not all regions on the aneurysm wall are experiencing such a large oscillation in WSS magnitude and direction; Figure 6.10 illustrates that the regions of high oscillation amplitude are very localized. In the case CH of patient C, time traces of WSS magnitude
and WSS vector angle at two points on the upstream aneurysm are plotted in Figure 6.10 (right). The WSS distribution shown in Figure 6.10 (left) is a snapshot at the systolic peak. The WSS magnitude at the point marked with letter ‘M’ changes from 0 to 10 N/m² over the cardiac cycle in phase with the flowrate profile. High frequency oscillations with magnitude 2 N/m² are superimposed on this slowly varying time trace of the WSS magnitude. The angle deviation, however, shows large oscillations from -160 to 180 degrees. The WSS vector at the point ‘L’ demonstrates the opposite behavior; it changes its direction significantly less (±5 degrees) during the cardiac cycle. The WSS magnitude, however, fluctuates rapidly with amplitude ±5 - 10 N/m² due to the flow instability; it also follows the flowrate profile varying from 10 N/m² at the diastole to 25 N/m² at the systolic peak.

Inside the aneurysm of patient B, the stagnation area exhibits a low WSS region surrounded by a band of high WSS as shown in Figure 6.11 (b) and (c). The low WSS region has higher pressure than the pressure in the adjacent walls by 1 mmHg. This pattern of WSS and pressure distribution agrees well with the experimental observations [71, 98] in which it is pointed out that the high WSS region surrounds the impingement point. This pattern of high/low WSS is also noted from the upstream aneurysm of patient C as shown Figure 6.10 (left). In this plot, the low WSS region at the aneurysm fundus looks larger than that of patient B, but the surrounding high WSS is clearly observed. More dramatic is the spatial change in direction of WSS vectors around this spot; all WSS vectors point outward in radial directions over the cardiac cycle. From this figure, it is clear that the flow impinges near the fundus of the aneurysm forming the stagnation point and creating a high WSS area around the impingement (stagnation) area. It is also interesting that this critical location moves around during the cardiac cycle; this is shown by the dots in Figure 6.11 (b) and (c), which correspond to the lowest WSS spot at instants marked with dots of the corresponding colors. Therefore, a WSS vector at a fixed point near the stagnation area changes its direction ‘temporally’ due to change in the impingement location over the cardiac cycle.

6.3.4 Flow structure inside the aneurysm

Next we examine temporal changes of global flow structures inside aneurysm such as the inflow/outflow regions and their changes along the depth are examined. We present the flow structure inside the aneurysm of case CH because case CH shows the strongest insta-
bility among the three patients. Figure 6.12 shows the distribution of velocity component normal (a-d) or parallel (h-l) to the plane on which data are extracted in case CH, VFR = 200 mL/min. The planes and time instants for the velocity computation are shown in Figure 6.12 (f-1,2 and g-1,2). The time interval between the time instants in Figure 6.12 (f-2) is close to the half period of the dominant velocity fluctuation. For comparison, black lines in Figure 6.12 (h-l) were drawn as a reference, which is the border between the positive and negative regions in Figure 6.12 (i).

Comparison of normal velocity distribution among Figure 6.12 (a) to (d) shows that negative (into the aneurysm) and positive (out of the aneurysm) regions do not change significantly over the cardiac cycle. Inside the aneurysm, the negative (inflow) region gradually moves toward the distal part of the aneurysm along the depth, following the aneurysm wall due to the inertia until it impinges the distal dome of the aneurysm. Although the flow is unstable as demonstrated in the time traces of velocity at history points in Figure 6.6, flow structures of positive and negative regions on planes over the cardiac cycle seem to change insignificantly. However, a closer look into the flow during the decelerating systole shows more changes as shown in 6.12 (h-l) marked with black arrows, i.e. a patch of negative region appearing in the positive territory, and the contour lines crossing the black border line; these small scale changes are not significant enough to change the global flow structure. While the velocity fluctuates inside the aneurysm, pressure also fluctuates near the wall with peak-to-peak magnitude about $100 \sim 200 \, \text{N/m}^2$ during the decelerating systole as shown in Figure 6.13 (c). Pressure increases locally near the outer neck of aneurysm wall, and a region of positive pressure difference $P_n - P_m$ is clearly shown in Figure 6.13 (a) while the flow rate is decreasing.

### 6.3.5 Statistics of wall shear stress

The WSS vectors with small magnitudes exist where the flow becomes stagnant and they are susceptible to large direction changes. In a straight pipe, the ratio of the average WSS to the maximum WSS, $R_{\text{wss}}$, in a pulsatile flow will have a similar ratio of the average VFR to the maximum VFR, $R_{\text{vfr}}$, when the Womersley number is small. A large Womersley number makes the ratio $R_{\text{wss}}$ smaller than $R_{\text{vfr}}$. The cases we simulated have complicated geometries far from a straight pipe. Hence, the ratio $R_{\text{wss}}$ becomes larger than $R_{\text{vfr}}$. Intuitively, the ratio $R_{\text{wss}}$ is thought to be different among different points. However, it turns out to
be close to a constant. In other words, the ratio $R_{wss}$ depends on the location but not a lot.

Relation between magnitude and direction of instantaneous WSS vector

The plots of direction change in WSS vector versus WSS magnitude reveal that as the WSS magnitude increases, the WSS vector deviates less from the reference state. Simulation results from the different cases of patient A, i.e. cases AL (VFR = 200 ml/min) and AH (VFR = 250 ml/min) listed in Table 6.2, are shown in Figure 6.14 as a representative case, since plots of other patients show similar patterns. It is noteworthy that most data points are gathered around the origin of the coordinate, which corresponds to low WSS magnitude and small angle change. In particular, 86% of the total points have less than 20 degrees in direction change and 66% of points are between 0 and 20 N/m² in WSS magnitude. When the VFR increases from 200 ml/min to 250 ml/min, the points disperse due to the WSS increase and flow instability, but the pattern remains essentially the same. The variation of this trend with respect to the location of sampling is shown in Figure 6.15 (right). For example, red points in Figure 6.15 (a) are sampled on the upstream aneurysm of patient C, and angle changes are plotted against WSS magnitude in Figure 6.15 (r-2). This figure is very similar to Figure 6.14 but other patches plotted in Figure 6.15 (b-2, y-2) show significantly different patterns. Plots of OSI versus WSS magnitude also show an inverse relationship between them. As the WSS magnitude increases, OSI decreases as shown in Figure 6.15 (c).

Relation between average WSS and maximum WSS

The average WSS and maximum WSS over the cardiac cycle shows a linear relation for all patients over a wide range of VFR 150 ∼ 350 ml/min. At a fixed point on the wall, the ratio of maximum WSS to average WSS is around 1.7 as the plots of patients B and C show in Figure 6.16. The blue (red) dots correspond to a lower (higher) VFR case in each patient. The increased VFR disperses the data points, increasing the maximum WSS as well. We also plot the maximum WSS versus the temporal average WSS on small patches, e.g. aneurysm, MCA/ACA bifurcation, and highly curved ICA segment as shown in Figure 6.15 (a). These plots show that this linear relationship still holds locally overall, although the flow instability increases the slope and scatters the points from a least-square fitting line for the case of aneurysm as shown in Figure 6.15 (r-1). If the entire domain is considered, the ratio (slope of the linear fitting line in the plot) is about 1.7, i.e., close to the ratio of
VFR at the systolic peak to the average VFR, 1.5, both in our simulation and also in [47].

### 6.4 Flow instability in the Circle of Willis (CoW)

Instability is observed in a blood flow simulation in the Circle of Willis. We have performed unsteady 3D flow simulations in a patient-specific geometry consisting of 34 arteries with a saccular aneurysm growing on the right ICA. The patient-specific inlet boundary conditions are given as follows. Mean velocity at the left ICA, right ICA, left vertebral artery, right VA are 0.291 (m/s), 0.290 (m/s), 0.212 (m/s) and 0.284 (m/s). The corresponding Womersley numbers at the four inlets (Left ICA, Right ICA, Left VA, Right VA) are 3.699, 3.457, 2.309, 2.338. The mean Reynolds number is 394 based on the mean velocity at the left ICA, the radius (R), and the kinematic viscosity.

The mean VFR on the left ICA is the highest among 4 inlets and the flow on the left ICA and ACA becomes unstable during the decelerating systole as shown in Figure 6.17. However, flow inside the aneurysm or in the right circulation network does not show any instability. The frequency spectrum is given in Figure 6.18 showing peaks at the frequencies similar to those found in aneurysmal flow cases.

### 6.5 Effect of compliant walls on the instability

As regards the assumption of rigid walls, it can possibly affect the magnitude of WSS and pressure and/or the spectrum of velocity/WSS fluctuations. From the reports of [136] and [108], we expect that our simulations with rigid walls may overestimate somewhat the WSS magnitude. However, as [136] demonstrated that the effect of the deformable walls in a lateral aneurysm case is not as significant as in the terminal aneurysm case, we estimate that wall compliance do change only slightly the flow structure and WSS distribution in our case. We have also performed two-dimensional simulations with compliant walls and found that the velocity time traces change by less than 10% over a 10-fold change in the elastic modulus of the wall. However, we have not performed full three-dimensional simulations and the rigid wall assumption is a limitation of this study requiring further investigation.

Flow in a channel of width 4 mm with flexible bottom wall. The wall at the top is fixed and the both ends of bottom wall is also fixed. The time traces of fluid velocity and solid displacements at several points are plotted in Figure 6.19. The flow is assumed to be
periodic and history points are marked with circles. The velocity fluctuation either amplifies or attenuates due to the compliant wall movement.

### 6.6 Discussion

Our study shows that flow instability may occur in certain saccular aneurysms but not in all aneurysms. Specifically, the narrow-necked lateral aneurysm of patient B does not show velocity fluctuations seen in other patients until the VFR reaches 400 mL/min which is beyond the physiologically correct VFR. This flow instability does not seem to be affected by flow rate changes in the bifurcations and small vessels as documented in our sensitivity study. Moreover, this study has not considered terminal aneurysms. Based on the fact that wide-necked aneurysms in patients A and C show much stronger velocity fluctuations from the VFR as low as 250 and 150 mL/min, we anticipate that flows in terminal aneurysms may be more susceptible to instability.

<table>
<thead>
<tr>
<th>Carreau</th>
<th>$\mu = \mu_\infty + (\mu_0 - \mu_\infty) \left[1 + (\lambda \dot{\gamma})^2\right]^{(n-1)/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda = 25s, n = 0.25$</td>
<td>$\mu_0 = 2.5P, \mu_\infty = 0.035P$</td>
</tr>
<tr>
<td>$\lambda = 3.313s, n = 0.3568$</td>
<td>$\mu_0 = 0.56P, \mu_\infty = 0.0345P$</td>
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<table>
<thead>
<tr>
<th>Carreau-Yasuda Model</th>
<th>$\mu = \mu_\infty + (\mu_0 - \mu_\infty) \left[1 + (\lambda \dot{\gamma})^p\right]^{(n-1)/p}$</th>
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</thead>
<tbody>
<tr>
<td>$\lambda = 1.902s, n = 0.22$</td>
<td>$\mu_0 = 0.56P, \mu_\infty = 0.0345P, p = 1.25$</td>
</tr>
<tr>
<td>$\lambda = 0.11s, n = 0.392$</td>
<td>$\mu_0 = 0.22P, \mu_\infty = 0.022P, p = 0.644$</td>
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<table>
<thead>
<tr>
<th>Ballyk Model</th>
<th>$\mu = \lambda(\dot{\gamma})((\dot{\gamma}))^{n(\dot{\gamma})-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda(\dot{\gamma}) = \mu_\infty + \Delta \mu \exp\left[-(1 + \frac{\dot{\gamma}}{a}) \exp(-\frac{b}{\dot{\gamma}})\right]$</td>
<td></td>
</tr>
<tr>
<td>$n(\dot{\gamma}) = n_\infty - \Delta n \exp\left[-(1 + \frac{\dot{\gamma}}{c}) \exp(-\frac{d}{\dot{\gamma}})\right]$</td>
<td></td>
</tr>
<tr>
<td>$n_\infty = 1, \Delta n = 0.45$</td>
<td>$\mu_\infty = 0.0345P, \Delta \mu = 0.25$</td>
</tr>
<tr>
<td>$a = 50, b = 3, c = 50, d = 4$</td>
<td>[74]</td>
</tr>
<tr>
<td>$n_\infty = 0.45, \Delta n = 0.45$</td>
<td>$\mu_\infty = 0.035P, \Delta \mu = 0.25$</td>
</tr>
<tr>
<td>$a = 70.71, b = 4.24, c = 70.71, d = 5.66$</td>
<td>[86]</td>
</tr>
</tbody>
</table>

Oscillations reported herein seem to be induced by a hydrodynamic instability that is described by the Rayleigh’s inflection condition [37]. Hydrodynamic instability and transition into turbulence in arterial pulsatile flow has been studied extensively in the past [103, 126, 39, 14]. More recently, high-resolution simulations were performed for stenosed carotids by [45, 85, 60]. In all cases, turbulence or temporal fluctuations were observed in...
the decelerating systole or near the end of systole. The observed frequencies, however, are much higher than the frequencies observed in the current work and intraoperative Doppler recordings of [126]. The reasons for the discrepancy seem to be the different flow conditions such as the much higher Reynolds number 1000-2000 of the flow in the aorta or the stenosed carotid. In the numerical study of flow over periodic grooves in a channel by [50], the frequency of the self-sustained oscillation corresponding to the least unstable Tollmien-Schlichting mode was predicted from linear stability analysis. Our peak frequencies of patient C (around 24 ~ 58 Hz) seem to agree well with a frequency range (16 ~ 24 Hz) found in their study; this frequency range corresponds to frequencies in grooves with non-dimensional separation distance $L = 5$ and non-dimensional groove length $l = 2.5$ with different depth (non-dimensionalized with the half-channel width). The Reynolds numbers in our study based on the flow rate and the kinematic viscosity are 877 and 1271 on average and at the systolic peak, respectively. They are in good agreement with the critical Reynolds number for the onset of instability which is close to $Re = 975$ [50].

Blood is a non-Newtonian fluid with shear-thinning and yield-stress. The effects of non-Newtonian property on the flow distribution in large arteries have been investigated and some studies show dramatic effects [52, 51] while others report a small effect limited to a fraction of the cardiac cycle [74, 110]. When the shear rates are higher than 50 or 100 s$^{-1}$ [90, 45], blood can be treated as Newtonian with constant viscosity. In our simulations, we assumed that the physiological flow rates in the ICA are in the range 200-250 mL/min, which gives an average velocity in the range of 0.265 ~ 0.331 m/s. This is based on the diameter of the ICA near the supraclinoid artery in our geometry, which is less than 4mm and the characteristic shear rate $8V_a/3r$, 353 ~ 441 (s$^{-1}$), where $V_a$ is the average velocity and $r$ is the radius of the blood vessel. We confirmed that even inside the aneurysm, the shear rates are well above 100 s$^{-1}$ even at the end of diastole. Our a posteriori analysis is shown in Figure 6.20 with three non-Newtonian models and two different parameters per model, which are summarized in Table 6.3. The characteristic shear rate $\sqrt{2tr(D)}$ where $D_{ij} = 1/2(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$, $i, j = 1, 2, 3$ [91] is above 100 s$^{-1}$ even at the end of diastole of a case with the smallest flow rate 150 mL/min except near the fundus of the downstream aneurysm and near the center of upstream ICA as shown in Figure 6.20 (top). For example, the shear rates at the black dots in Figure 6.20 (middle) are 1352 s$^{-1}$ and 1154.8 s$^{-1}$ for patient A and C, respectively. We also calculate the ratio, $\mu/\mu_N$, of apparent viscosity ($\mu$) using the
three non-Newtonian models, i.e., the Carreau, Carreau Yasuda, and Ballyk models, to the Newtonian viscosity ($\mu_N$) used in our simulations as shown in Figure 6.20 (middle). Except the center of the aneurysm of patient A and of the parent vessels of patient C, the shear rates are well above $200 \, \text{s}^{-1}$ and the apparent viscosity is close or smaller than what is used in the present study. Hence, we expect that the Newtonian assumption is acceptable in our simulations as it will not affect the onset of flow instability.

Our current study shows that the impingement locations inside aneurysms exhibit dynamically changing patterns of high or low shear and high static pressure as well as temporal oscillations in the direction of WSS vectors. Hence, the oscillatory behavior of WSS vectors at such critical locations inside aneurysm may be an important factor that should be considered for the pathology of an aneurysm. We have not attempted yet to establish a model which would represent the effects of flow on aneurysm development, or of systemic hypertension. In order to understand such pathological interactions between unsteady flow and aneurysms, the aggregation of red blood cells or adhesion of white blood cells and platelets to the aneurysmal wall has to be simulated in detail. However, the existing non-Newtonian models are inadequate in modeling the discrete nature of the blood rheology inside the aneurysm. Ultimately, we aim to assess the effects of non-Newtonian behavior and elastic wall from ‘atomistic’ models (i.e., discrete at the scales of active entities such as cell adhesion molecules) and not from continuum-level phenomenological models. Hence, it seems necessary to develop a new multiscale methodology to simulate the interaction of the unsteady flow with the blood cells and quantify their aggregation, accumulation or adhesion to endothelial wall inside the aneurysmal cavity. To this end, we are developing a hybrid continuum-atomistic formulation on two overlapped domains, with the latter employed in a small domain that includes the aneurysm while the former employed in a much larger domain to represent accurately the large-scale flow dynamics. The atomistic formulation is based on the Dissipative Particle Dynamics method whereas the continuum method is based on the incompressible Navier-Stokes equations using the spectral element method [40].

6.7 Conclusions

Through a series of highly-resolved CFD simulations, aneurysmal flow in wide-necked saccular intracranial aneurysms is shown to exhibit instabilities in the VFR 150-250 mL/min,
which is lower than the mean VFR is 275 mL/min with standard deviation ±52 mL/min [47]. Flow in a narrow-necked lateral aneurysm becomes unstable as the VFR in the ICA reaches 400 mL/min. Specifically, we observed that the pulsatile flow in aneurysms is subject to a hydrodynamic instability during the decelerating systolic phase resulting in a high-frequency oscillation over that period [126]. The flow returns to its original pulsatile state near the end of diastole. The frequency of velocity fluctuations in our simulations ranges from 20 to 50 Hz, and is in good agreement with the Doppler frequency recordings [126]. Inside saccular aneurysms, the pattern around the impingement areas shows relatively high static pressure and low WSS region surrounded by a band of higher WSS. At such locations, the WSS vectors are spatially changing significantly in their direction. Due to flow instability, the WSS vectors fluctuate in magnitude and direction. In stagnation regions, the pressure/WSS patterns also fluctuate and move around spatially. The temporal change in these locations increases the temporal variation of WSS vectors. The oscillatory behavior of WSS vectors, in combination with high/low WSS magnitude and locally elevated static pressure in stagnation areas, may play an important role in the formation and rupture of an aneurysm.
Figure 6.1: Geometric models of patients A (left), B (middle), and C (right) defined in Table 6.1. The second row shows zoom-in of aneurysms indicated by blue circles in the top row. The blue lines indicate the center of the supraclinoid ICA segment, which is the region of interest in this study, harboring aneurysms in patients A, B, and C. Colors represent $z$-coordinates for viewing clarity. All shown arteries are on the left from the median plane and aneurysms are located at the level of eyes and below the right ventricles and above the intracranial base. ‘L’, ‘P’, and ‘S’ denote lateral (x), posterior (y), and superior (z) directions, respectively. Third row shows surface elements and elements with quadrature points in a cut marked with rectangles in the first row. Fourth row shows the volumetric flow rate profile over the cardiac cycle at different average volumetric flow rates, 150, 200, and 250 mL/min.
Figure 6.2: Patient A (case AH, VFR = 250 mL/min): (a) Streamlines in the aneurysm. Yellow ribbon streamlines show swirling flow which starts from the bottom of the aneurysm and rises up along the center of the aneurysm. (b) Contour plot of $y$-component of velocity at a plane at the systolic peak. The black line A-B and the adjacent arrow indicate the location of velocity measurement and direction of increasing $y$ for plotting in (c), respectively. (c) Velocity components $U$, $V$, and $W$ at the black line shown in (b) are plotted. $U$, $V$, and $W$ denote $x$ (lateral), $y$ (posterior), and $z$ (superior) components of fluid velocity, respectively.
Figure 6.3: Patient C (case CL, VFR = 200 mL/min) : (a) The three lines (two vertical lines ‘R’ and ‘K’ and one horizontal line ‘M’) and adjacent arrows show the locations of sampling and increasing direction of \( x \) or \( y \) coordinates, respectively. (b) VFR profile showing two instants of the velocity computation along the lines in (a). The two instants are marked with parenthesized letters, ‘c’ and ‘d’. (c-1, 2) show profiles of centerline velocity along the three lines ‘R’, ‘K’, and ‘M’ at the systolic peak. (d-1, 2) show profiles of centerline velocity along the three line ‘R’, ‘K’, and ‘M’ at an instantaneous time during the decelerating systole. X(L), Y(P), and Z(S) denote lateral, posterior, and superior directions, respectively.
Figure 6.4: Patient A (case AH, VFR = 250 mL/min): Velocity time traces at four history points. Right bottom shows the plot of VFR versus time within the third cardiac cycle. The oscillations start during the decelerating systole. A case VFR = 150 mL/min is shown for comparison purposes. X(L), Y(P), and Z(S) denote lateral, posterior, and superior directions, respectively.
Figure 6.5: Patient B (case BH, VFR = 350 mL/min): Velocity time traces at history points with volumetric flow rates at the PCoA and the ophthalmic artery and the MCA over the cardiac cycle at different outflow boundary conditions. Black solid and red dotted lines correspond to constant pressure and RC-type outflow boundary conditions, respectively. Pt 5 is upstream of the aneurysm. Pt 1, 3, and 6 are downstream of the aneurysm. All other points are inside the aneurysm. X(L), Y(P), and Z(S) refer to lateral, posterior, and superior directions, respectively. ‘RC’ and ‘CP’ refer to RC-type and constant pressure outflow boundary conditions, respectively.
Figure 6.6: Patient C (case CL, VFR = 150 mL/min): Time traces at history points inside the aneurysm for velocity convergence test. U, V, and W components at Pt 1 and Pt 10 are plotted on the right and the time-dependent flow rate is also plotted for phase comparison. The red boxes show the time interval where the velocity and WSS errors are measured among different polynomial orders. U, V, and W denote x (lateral), y (posterior), and z (superior) components of fluid velocity, respectively.
Figure 6.7: Power spectral density of velocity-time traces at different history points for cases AH, BH, and CL. Pt 10 of patient B is located near the fundus of aneurysm. Points, Pt 14 and Pt 15 in patient A, and Pt 1 in patient C, are shown either in Figure 6.4 or in Figure 6.6. Pt 10 of patient B is similar location with Pt 1 of patient C; both are near the fundus of the corresponding aneurysm. The lower plot shows the changes in spectra at Pt 14 of patient A as the average VFR increases from 150 mL/min to 250 mL/min.
Figure 6.8: Patient A (case AH, VFR = 250 mL/min): Left top shows the regions where WSS vectors are calculated; each region has two discrete points corresponding to the two curves in each plot. Time traces of magnitude and direction of WSS vectors at each point are shown for each region ‘L’, ‘M’, and ‘N’. The angle of a WSS vector is calculated with reference to corresponding WSS vectors at the systolic peak. WSS time traces at VFR = 150 mL/min are shown for comparison purposes.
Figure 6.9: Patient C (case CH, VFR = 200 mL/min) : Contour plot of WSS magnitude and WSS vectors on the left, and time traces of the magnitude and direction change of WSS at two points, ‘L’ and ‘M’, on the wall. Left: Two points for computations of WSS magnitude and angle are marked with red dots labeled ‘L’ and ‘M’. The solid yellow lines show the locations of the converging and diverging lines at the current instant while the dotted yellow lines next to them indicate how far these stagnation lines move over the cardiac cycle. Right: Time traces of WSS magnitude and angle changes at points ‘L’ and ‘M’. The units of magnitude and direction are \( \text{N/m}^2 \) and degrees, respectively. The left bottom plot shows the flowrate profile and the red dot indicates the instant when the left snapshot was taken. X(L), Y(P), and Z(S) refer to lateral, posterior, and superior directions, respectively.
Figure 6.10: Patient C (case CH, VFR = 200 mL/min): WSS magnitude and direction change at two points with contrasting characteristics on the upstream aneurysm at the systolic peak as marked with a red dot on the right bottom plot of VFR. Left: WSS vectors on the contour plot of WSS magnitude at the distal dome of the upstream aneurysm at the time indicated in cycles. Two history points are marked with red dots labeled ‘L’ and ‘M’. Right: Corresponding time traces of the WSS magnitude and direction change. The units of magnitude and direction are $N/m^2$ and degrees. The left bottom plot shows the flowrate profile over the cardiac cycle. X(L), Y(P), and Z(S) refer to lateral, posterior, and superior directions, respectively.
Figure 6.11: Patient B (case BL, VFR = 350 mL/min) : WSS vectors around the impingement (stagnation) point inside the aneurysm. (a) Locations of high OSI; ‘OSI1’, ‘OSI2’, and ‘OSI3’. X(L), Y(P), and Z(S) refer to lateral, posterior, and superior directions respectively. (b) Plot of WSS magnitude and WSS vectors around the region ‘OSI1’ at the systolic peak. (c) Plot of WSS magnitude and WSS vectors around the region ‘OSI1’ at an instant during the decelerating systole, which is marked with the red dot on the left bottom VFR plot. The dots show the instantaneous locations of the center of the stagnation point at times marked with the dots of the same color at the left bottom VFR plot.
Figure 6.12: Patient C (case CH, VFR = 200 mL/min): Distribution of normal or parallel velocity on a plane cutting through the aneurysm. In (a)-(d), positive velocity means flow out of the plane, showing inflow and outflow. In (h)-(l), positive means flow along the direction marked with the pink arrow in (i). This plane is taken at the neck and near the fundus of the aneurysm as shown in (g-1,2). (a)-(d) show the normal velocity distribution at different phases of the cardiac cycle from the dicrotic peak, end of diastole, systolic peak, and decelerating systole, respectively. (a, h) Letters, ‘O’, ‘I’, ‘D’, and ‘P’, indicate the locations of the outer side of the bend at the upstream aneurysm, of the inner side of the bend at the upstream aneurysm, of the distal portion of the aneurysm, and of the proximal portion of the aneurysm, respectively. ‘L’, ‘P’, and ‘S’ denote lateral, posterior, and superior directions, respectively. (f-1,2) and (g-1,2) show the time instants when the velocity fields are taken. Bottom (h)-(l) show distribution of centerline velocity on the plane cutting through the aneurysm near the fundus of the aneurysm at five time instants marked with red dots at (f-2). Black lines in (h)-(l) mark the border line between positive and negative regions of (i). The black arrows in (j) and (l) mark the area where changes from (i) and (k) are pronounced.
Figure 6.13: Patient C (case CH, VFR = 200 mL/min): (a) Distribution of pressure difference, $P_n - P_m$ at time instants marked with circles on the right bottom (c). (b) Volumetric flow rates over the cardiac cycle. (c) Time trace of pressure at a point indicated by an arrow on the left (a) during the time interval marked with a box in (b).
Figure 6.14: Patient A: Statistical plot of WSS vector direction change versus WSS magnitude for cases AL and AH presented for all lumen points and for all times during the third heartbeat. Each point represents WSS and direction change at an instantaneous time and a fixed point on the wall. Red dots represents a case of higher VFR (AH, 250 ml/min) than blue dots (case AL, 200 ml/min). Some blue and red points overlap, thereby masking the red close to the axes.
Figure 6.15: Patient C (case CL, VFR = 150 ml/min): Plots of maximum WSS versus average WSS, shown on the right for regions of the points where the computations are performed, shown on the left. (a) The points on the wall where the WSS magnitude and angle deviation from a reference WSS vector is computed. The colors match with the plots on the right (r-1,2), (b-1,2), and (y-1,2). Regions labeled as y, r, and b correspond to the MCA/ICA bifurcation, the upstream aneurysm, and the lacerum ICA segment, respectively. (r-1, y-1, b-1) Plots of maximum WSS versus average WSS in the region r, y, and b, respectively. (r-2, y-2, b-2) Plot of angle changes of WSS vector versus WSS magnitude in the region r, y, and b, respectively. (c) Plot of WSS magnitude versus OSI in the entire domain.

Figure 6.16: Patient B (left) and C (right): Plots of maximum WSS versus average WSS. Each point represents average WSS and maximum WSS over the cardiac cycle at a fixed point on the wall. Red dots represent a case of higher VFR (case BH and CH) than blue dots (case BL and CL) for each patient B and C. The slopes of the least-square fitting lines are 1.70 for all cases.
Figure 6.17: Comparison of time traces of velocity at history points between aneurysm model and a hypothetical model with aneurysm removed. (a) Geometry of intracranial arterial network. (b) shows the time traces of volumetric flow rates at the right ICA and left ICA. (c) shows the time traces of the volumetric flow rates at the right VA and left VA. More than 50 history points are located in the ICA and around in the Circle of Willis. Three of them are marked with numbers and arrows in (a). History pt 1, pt 2, and pt 3 are located at the anterior communicating artery, the left anterior cerebral artery, and the left supraclinoid ICA.

Figure 6.18: Plot of time traces (left) and Fourier spectrum (right) of velocity at a history point in the left ACA in the brain circulation. (left) Time traces of velocity at history pt ‘2’ in Figure 6.17 and volumetric flow rate at the left ICA. (right) Fourier spectrum of velocity time trace in the left. Right bottom figure shows the zoomin of top Fourier spectrum.
Figure 6.19: Velocity and displacement time traces at two pink points marked with arrows are plotted. The bottom wall including the aneurysm sac is assumed to be linear elastic. ‘E1’, ‘E2’, and ‘E3’ correspond to Young’s Modulus 20 kPa, 30 kPa, 50 kPa, respectively. ‘Pt 13’ shows the time trace of displacement of the wall and ‘Pt 25’ shows the time trace of mesh velocity at the fluid-structure interface. Other ‘Pt 23, 0, 28, 11, 10’ show the time trace of fluid velocity.
Figure 6.20: Shear rate isocontours lower than 100 s$^{-1}$ at the end of diastole of patient A (left) and C (right). The ratio of apparent viscosity using Carraeu-Yasuda 1 [25] case to the Newtonian viscosity used in the simulations from the flow fields at the end of the diastole of patient A (left) and of patient C (right). Isosurfaces were extracted at the viscosity ratio 1.1. Bottom: plot of apparent viscosity $\mu$ versus shear rate ($\dot{\gamma}$) ‘Carreau 1’ and ‘Carreau 2’ refer to Carreau model used in [86] and [25], respectively. ‘Carreau Yasuda 1’ and ‘CarreauYasuda 2’ refer to Carreau-Yasuda model used in [25] and [52], respectively. ‘Ballyk 1’ and ‘Ballyk 2’ refer to Ballyk model used in [74] and [86], respectively.
Chapter 7

Flow in Infundibular Bifurcations

7.1 Clinical motivation

The PCoA origin is located along the posterior wall of the the supraclinoid internal carotid artery (ICA), and is one of the most common sites for intracranial aneurysms [106]. The infundibular origin of the PCoA is a common variant seen in approximately 5% to 17% of patients [106, 83]; other researchers [116, 38] report a higher incidence of 7% to 25%. Multiple intracranial aneurysms and aging further increase the chance of incidence [116, 113]. There are several reports on growing aneurysms on the widened infundibular PCoA branch [129, 73] as shown in Fig. 7.1 (right). Moreover, there have been a number of case reports on the progression of funnel-shaped PCoA origin to aneurysm formation and subsequent rupture leading to subarachnoid hemorrhage (SAH) [96, 109]. Jang et al. [73] also reported a case of ruptured aneurysm harboring on the distal wall of infundibular PCoA and they also summarized twelve cases they found through literature review. More recently, Coupe et al. compiled six case reports of SAH from infundibular rupture in patients aged between 40 and 57 [27]. Those infundibular ruptures were located in either the right or left PCoA. In other words, widened infundibula, even without any growing aneurysm on them, may rupture and result in SAH and fatal conditions [105]. Rupture of a bulge at the distal junction of the right ICA and the PCoA was reported by Kuwahara et al. [83], the root of which was enlarged to the extent that it looked like an aneurysm. The need to monitor the patients with infundibula which might lead to aneurysm formation and rupture was emphasized by Cowan et al. [28].

Flows in aneurysms have been studied experimentally [84, 71] and also through computer
simulations [127, 20]. Aneurysmal flow have been studied with emphasis on high or low WSS regions and flow impinging areas inside aneurysms [23, 119, 24, 132, 138]. Impinging zones and areas of high WSS were correlated to aneurysm rupture [22]. The histological study of Meng et al. [98] also shows that destructive remodeling involving loss of smooth muscle cells occurs at the region of high WSS and WSS gradient, where the flow accelerates near the impinging area. Therefore, we examine the flow pattern in the infundibulae, WSS/pressure distributions in the PCoA region, and the effect of widened root of a branch on the impinging patten using patient-specific infundibulum and aneurysm geometries. In addition to constructing anatomically correct models, we also created some hypothetical models to investigate the effect of enlargement at the root of a branch on the WSS/pressure distribution. While there have been many computational studies of aneurysms, it seems that our computational study with a patient-specific infundibulum is the first attempt. In particular, we investigate WSS/pressure, the direction of WSS vectors at an infundibulum, the change of WSS/pressure distribution when an aneurysm grows at the root of a branch, and finally the flow instability.

This chapter is organized as follows. In section 7.2, we present the geometrical models used for simulations, simulation parameters, and boundary conditions. In section 7.3 we present simulation results followed by a discussion in section 7.4.

Table 7.1: Dataset for 3D patient-specific models. The units of image size and resolution are voxles and $10^{-3} \text{mm/voxel}$, respectively. CTA: Computer Tomography Angiography. DSA: Digital Subtraction Angiography. ‘Ane.’ and ‘Inf.’ are abbreviated forms of aneurysm and infundibulum, respectively.

<table>
<thead>
<tr>
<th>Patient</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
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<td>Inf. and Ane.</td>
<td>Ane.</td>
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</table>

7.2 Methods

Institutional Review Board (IRB) approval was obtained for this retrospective review. Records of CT Angiography (CTA) performed for intracranial aneurysms of many patients were reviewed over a 12 month period. Four patients (A-D) listed in Table 7.1 were selected
for this study having different types of PCoA bifurcations: infundibulum (A); infundibular bifurcation and aneurysm growing at the neck of the infundibulum (B); single saccular aneurysm at the root of the PCoA (C); two wide-necked aneurysms in proximity at the PCoA root and downstream (D).

To generate patient-specific geometries for computation, an in-house Matlab (The Mathworks, Natick, MA) tool in combination with Amira (Visage Imaging, Andover, MA) were used to capture and export isosurfaces based on the intensity of computer tomography angiography (CTA) or digital subtraction angiography (DSA) datasets of four patients. Then, using Gridgen (Pointwise, inc. Fort Worth, TX), a front-tracking mesh generation tool, we created smooth surface models which consist of small surface patches. The final geometries with extruded inlet and outlets are shown in Figs. 7.1, 7.2, and 7.3. We also removed the aneurysms from patients C and D to create hypothetical aneurysm-free models. We described the manual editing procedure in detail in Chapter 2. A total of seven geometric models from four patients were generated.

Patient A has a PCoA infundibulum as shown in Fig. 7.1 (left). It is worth mentioning that the aneurysm grows at the bend of the cavernous ICA segment far upstream of the infundibulum. Patient B in Fig. 7.1 (right) has an aneurysm growing at the junction of the ICA and the infundibulum. The large anterior choroidal artery (AChA) is also noticeable; although it is not funnel-shaped, we expect that a somewhat similar WSS/pressure distribution pattern is established in this bifurcation. Patient C in Fig. 7.2 has an aneurysm with a daughter lobule at the root of the PCoA. The PCoA starts from the proximal aneurysm wall and turns around almost 180 degree, making a sharp bend. Patient D in Fig. 7.3 has two aneurysms in the supraclinoid ICA segment, located between the PCoA root and ICA bifurcation into the middle cerebral artery (MCA) and the anterior cerebral artery (ACA). One aneurysm grows at the root of PCoA and the other one is located within a short distance from the first aneurysm.

Using the patient-specific aneurysms in Figs. 7.2 (right) and 7.3 (right), we also created aneurysm-removed (hypothetical) models. Hypothetical models were generated by replacing the entire aneurysm with a slightly funnel-shaped infundibulum for aneurysms in bifurcation or a smooth surface patch for aneurysms without a branch as shown in Figs. 7.2 (left) and 7.3 (left); see Chapter 2 for more details of the procedure. The reason for creating such aneurysm-removed models is to quantify the changes in pressure and WSS distribution
pattern due to the presence of aneurysms, i.e., to investigate the effect of aneurysm growth on the flow. Here, we do not imply that hypothetical models have progressed into the aneurysms. However, we expect that such hypothetical models will shed some light on the effect of widening root of the bifurcation on WSS/pressure distribution, which is one of the objectives in this study. Hence, we do not present any extensive results of simulations with hypothetical infundibulum models except the comparison of WSS/pressure distribution between the original aneurysm and the hypothetical infundibulum models.

### Table 7.2: Simulation parameters.

The Reynolds number, Re, is based on the diameter of the inlet, mean velocity, and kinematic viscosity. The Womersley number, $\omega_n$, is based on the radius ($R$) of the inlet, pulsatile circular frequency ($\omega = 2\pi f$), and kinematic viscosity ($\nu$). ‘Lac.’, ‘Pet.’, and ‘Cer.’ are abbreviated forms of the Lacerum, Petrous, and Cervical ICA segment, respectively.

<table>
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<th>BA</th>
<th>CI</th>
<th>CA</th>
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</table>

With these seven models, blood flow was simulated in the ICA, the MCA, and the ACA. Based on WSS sensitivity studies on aneurysms in the supraclinoid ICA [18, 101, 107, 4], sufficiently long parent vessels are included in the computational domains at high Reynolds numbers with high volumetric flow rate (VFR) in order to avoid the inlet boundary effect. In all simulations listed in Table 7.2, the vessel walls are rigid and the blood is assumed to be incompressible Newtonian with kinematic viscosity $3.80 \times 10^{-6} \text{ m}^2/\text{s}$ due to the prohibitively high computational cost of deformable walls or Non-Newtonian fluid models. These limitations are addressed in the last section. The inflow condition is given by the time-dependent Womersley profile with specified VFR, which is the exact solution of flow in a rigid pipe under pulsatile pressure gradient. The VFR profile was taken from the measurements of Marks et al. [94], and eight complex Fourier coefficients were employed to calculate the Womersley profile during simulations; also, 80 beats per minute (BPM) were used in all simulations for the heart periodic pumping. The flow at the outlet boundaries are assumed to be fully developed flows, i.e. $\frac{\partial u}{\partial n} = 0$. 
In order to get physiologically correct pressure distribution, the pressure at the outlet vessels should be measured and imposed numerically or the flow rate and pressure relation has to be established [58], both of which are not available in most cases. Hence, constant pressure is used for the pressure boundary conditions at the outlets [20]. Windkessel or its variants, or impedance boundary conditions are used when the flow division is important in arterial systems with multiple outlets [137, 45, 124].

When flow division - such as in the Common Carotid Artery bifurcation - is considered, constant pressure is not a good choice because flow divisions at bifurcations are determined only by the resistance of the downstream vessel segment in the computational domain. In this study, however, our region of interest, i.e. the supraclinoid ICA where the PCoA begins, is upstream of the bifurcation and the WSS/pressure distribution is not affected when the ratio of flow rates in the MCA and ACA changes substantially [20]; see the Chapter 3 for a comparison between different outflow conditions. Hence, constant pressure boundary condition is employed in most simulations. Another type, the so-called “RC boundary condition” [58] is imposed for patient A and B to limit the flow rate at the PCoA because the average flow rate in the PCoA is less than 5 % of that in the ICA when the Circle of Willis is complete (49 % of cases) [2]. The RC boundary condition used in this study relates the pressure and the flow rates through the differential equation

$$P(t) + \frac{RC}{dt} = Q(t)R,$$

where $P(t)$, $R$, $C$, $Q(t)$ are the pressure at the boundary, the resistance, the capacitance, and the flow rate, respectively. Since the pressure is determined uniquely within a constant in the Navier-Stokes equations, a constant pressure or computed pressure from the flowrate is taken as a reference pressure in order to obtain a physiologically reasonable pressure in the computational domain.

The distribution of WSS and pressure under the pulsatile flow condition were examined by solving the Navier-Stokes equations with the parallel NEKTAR, which implements the high-order spectral/hp method. The NEKTAR code has been used and validated for many different bioflows, e.g. see [121]. This solver employs a high-order splitting scheme and each time step is composed of three substeps. At the first substep, the solver updates explicitly the previous time step solution with the nonlinear convection contribution. Then, the pressure is obtained by a Poisson equation using the updated intermediate velocity and Neumann pressure boundary conditions. At the third substep, the velocity is obtained by solving three inhomogeneous Helmholtz equations. The unknowns, i.e. velocity and
pressure, are expressed as a linear combination of a Jacobi polynomial basis, and $C^0$ continuity is imposed at the boundary of the elements. For more details of the method and implementation, we refer the reader to [77].

In our simulations, we monitor OSI which is defined as $\frac{1}{2}(1 - \frac{\int \int R^{\|}d\tau\|}{\int R^{\|}d\tau})$, where we denote the WSS vector by $\vec{\tau}$ and the integrations are done over the cardiac cycle. The WSS vector $\vec{\tau}$ is defined by a projection of the traction vector $\mu_N(\nabla u + \nabla^T u) \cdot n$ onto the tangent plane, and $\mu_N$ and $n$ are the Newtonian viscosity and the inward normal vector at the blood vessel wall, respectively. Simulations were performed for two to three cycles, and the data from the last cycle were used for comparison and further analysis. In our simulations, we found that aneurysmal flows tend to become unstable due to shear layer instability resulting in temporal fluctuations of velocity and WSS. In order to show that fluctuations in the velocity and WSS vector are not numerical artifacts, we carried out a thorough resolution study, i.e. $p$-refinement tests with the spectral/hp element method (see Chapter 3).
7.3 Results

7.3.1 Patient A: Infundibulum at the PCoA with a far-upstream aneurysm

Both cases AL (VFR = 250 ml/min) and AH (VFR = 300 ml/min), see Table 7.2, show very similar pattern of WSS/pressure distribution except that in case AH the WSS magnitude is increased by 10-20% due to higher flowrate. Here, we present results mainly from the case AH.

A snapshot of WSS/pressure distribution at the systolic peak in the infundibulum is shown in Fig. 7.4. A band of high WSS of 25-30 $N/m^2$ surrounds a low WSS location of 5 $N/m^2$. At the tip of the infundibulum, a sharp V-shaped turn of the PCoA creates another high WSS spot with magnitude 45 $N/m^2$. At the distal wall of the infundibulum, a high pressure region is marked with a pink arrow in Fig. 7.4 (middle left). This spot has higher pressure than the adjacent walls by 0.8 ∼ 1 mmHg. This slightly higher pressure location coincides with the aforementioned low WSS spot and the rupture location of infundibulae in the previous case reports [96, 109, 83, 105, 105]. The directions of WSS vectors in this region are spatially changing across the pink line in Fig. 7.4 (middle right). The spatial changes of average WSS vectors around the infundibulum, seen from a different viewpoint, are also shown in Fig. 7.5 (c). This figure shows more clearly that the flow impinges on the distal wall and spreads outward in the radial direction. The flow entering the infundibulum either swirls up and joins the blood stream, or forms a stagnation zone of WSS less than 1 $N/m^2$ at the proximal part of the infundibulum marked with a black arrow in Fig. 7.4 (bottom). This stagnation zone is characterized by high OSI and low WSS as shown in the circles in Fig. 7.5. When the WSS magnitude is plotted against OSI at each point on the wall, as shown in Fig. 7.5 (d), an inverse relationship is revealed.

Temporal average of WSS and maximum WSS were recorded during one period of the cardiac cycle at several points on the vessel walls. Corresponding plots are shown for both cases AL and AH in Fig. 7.6. They show a linear relationship with proportionality coefficient 1.7 even though the coefficient may vary depending on the location of sampling, as shown in Fig. 7.7. For example, as expected, the points at the aneurysm wall are scattered more and correspond to a coefficient 1.9, which is higher than the other regions. Also, at higher flowrate (VFR 300 ml/min, case AH), they spread out from the least-square fit line and show a weaker linear relation than at the lower VFR 250 ml/min. This spreading is due
to the stronger instability developed in the flow for case AH, as we will discuss in section 7.3.4. The ratio of peak VFR to average VFR in the ICA ranges from 1.43 to 1.48 in our simulations. The corresponding ratio 1.7 of the WSS magnitude is higher than simply the ratio of VFR due to the effect of complicated geometry and disturbed flow.

7.3.2 Patient B: Aneurysm growing at the neck of the Infundibulum

The distal neck of AChA bifurcation shows similar patterns of high pressure at the impinging point and high WSS around this point. Specifically, the high WSS (20 N/m$^2$) region at the root of the AChA is marked with a pink arrow in Fig. 7.8 (a). Above this spot, there exists a location of low WSS (less than 5 N/m$^2$) but high pressure (1 mmHg higher than the adjacent walls), marked with a pink arrow in Fig. 7.8 (b). These patterns of WSS and pressure at the distal neck of the root of the AChA bifurcation, however, are not as pronounced as they are in the infundibulum of patient A, because this AChA bifurcation is not funnel-shaped and the impinging flow to the AChA is disturbed due to the proximity of the upstream aneurysm at the PCoA.

The aneurysm of patient B is located at the distal neck of the PCoA infundibulum. We note that this location is about the same as the location of high pressure and surrounding high WSS band at the infundibulum of patient A and at the root of AChA. Close views from the opposite side of the aneurysm are shown in Fig. 7.8 (c-d). These two plots show a high WSS spot at the neck of the aneurysm and a high pressure area above the neck; both regions are marked by the pink arrows and the aneurysm neck is marked with pink dotted lines in Fig. 7.8 (c-d).

Flow visualizations show that the flow pattern inside the aneurysm of patient B is very similar to the description in the glass model experiment of Imbesi et al. [71]: the flow separates at the sharp corner, i.e. the neck of the aneurysm, and the separated flow impinges the distal aneurysm wall near the bottom of the aneurysm. The location of the high velocity cores moves along the depth of the aneurysm from the impinging side to the distal part of the aneurysm as marked with black arrows in Fig. 7.8 (e). Due to this aneurysmal flow, high WSS regions are observed on the aneurysm wall as shown and marked with black arrows in Fig. 7.8 (a).
7.3.3 Patient C with single aneurysm and patient D with two aneurysms in proximity

Comparison between the aneurysm-laden model (CA) and the aneurysm-removed model (CI) of patient C shows that the aneurysm does not reduce the high WSS/pressure found in the bifurcation but shifts and expands a high pressure spot (4-5 mmHg higher than the adjacent walls) and a high WSS band (50-60 \( N/m^2 \)) downstream, as shown in Fig. 7.9.

For patient D, changes in pressure distribution at the systolic peak are shown in Fig. 7.10 when aneurysms are formed. In all three cases, i.e. DI, DO, and DT, there exist locally elevated pressure regions (1-2 mmHg higher than the adjacent walls). In cases DO and DT, however, high pressure spots are shifted from the distal wall of the infundibulum to the neck of the upstream aneurysm. Other high pressure locations (0.8 mmHg higher than the adjacent walls) are formed at the distal dome of the aneurysm. WSS peaks (60-70 \( N/m^2 \)) get even higher at the distal neck of the aneurysms. Hence, the pattern of change in WSS/pressure distribution is consistent with that of patient C.

Inside the aneurysms of both patients C and D, a second impinging point is formed. The upstream aneurysm of patient D has locally elevated pressure spots at the distal dome tip. A similar phenomenon is seen in patient C, where the location of stagnation region due to the impinging coincides with the location of the daughter lobule.

7.3.4 Velocity fluctuations in aneurysms

Our results show that at some locations the velocity fluctuates in cases AL, AH, DO, and DT. In particular, case AH (patient A at VFR = 300 ml/min) shows that velocity fluctuations start at the bend where an aneurysm is located and during the decelerating systole as shown in Fig. 7.11; the plots of power spectral density changes along the vessel confirm that the fluctuations are becoming stronger near the infundibulum, as shown in Fig. 7.12.

More specifically, velocity time traces at Pt 16 and Pt 15 in Fig. 7.11 show the dramatic changes in the flow field from regular to irregular, i.e. from a velocity field following a smooth pulsatile flowrate to a fluctuating flow. These two points, i.e. Pt 16 and Pt 15, are located at the upstream and the downstream of the bend, respectively, where the aneurysm grows. It is clear that fluctuations in the velocity field start in the aneurysm and propagate
downstream. The fluctuations become stronger as the flow approaches the infundibulum. The high frequency components of the velocity profile at a downstream point (Pt 11) do not decay as fast as they do in the upstream points, e.g. Pt 16 and Pt 15, as shown in Fig. 7.12.

The frequency range of the three cases AH, DO, and DT are in good agreement with the Doppler recordings of Steiger and Reulen [126] as well as the fact that flow instabilities start during the deceleration phase and that the flow returns to smooth pulsatile state either at the end of the systolic deceleration phase or at the end of diastole. Inside the aneurysms of patient D, velocity time traces show fluctuations of relatively high frequency 30 - 40 Hz, as shown in Fig. 7.13, which is about 30 times the heart beat frequency \( f_{\text{heart}} = 1.25 \). The same oscillation is observed inside the aneurysm of case DO. However, it is one order lower than the frequencies of bruit reported by other clinicians and researchers [117, 123].

Oscillations reported herein seem to be induced by hydrodynamic instability. Visualization of the flow at the upstream aneurysm of patient D shows that the flow separates at the proximal neck of the aneurysm with the separated flow forming a shear layer, which is unstable and triggers the observed fluctuations [115]. A numerical study of flow over periodic grooves by Ghaddar et al. [50] gives a frequency range \( 16 \sim 24Hz \), which is close to the frequency range in patient D (aneurysms in patient D are assumed to correspond to grooves with non-dimensional separation distance \( L = 5 \) and non-dimensional groove length \( l = 2.5 \)). The Reynolds numbers in case DT, 877 and 1271 on average and at the systolic peak, respectively, are also around the critical Reynolds number for the onset of instability, 975, where the Reynolds number is based on the flow rate and the kinematic viscosity [50].

Due to the fluctuations in velocity, both the magnitude and direction of WSS vectors fluctuate in case AH. Figs. 7.11 (f) and (g) show time traces of WSS vectors at two points marked as ‘WSS1’ and ‘WSS2’ in Fig. 7.11 (a). Both points show WSS fluctuations both in magnitude and in direction during the decelerating systole and the distole. The point ‘WSS1’ is located at the band of high WSS marked with a pink line in Fig. 7.4 (top right). Hence, the maximum WSS magnitude is as high as \( 30 \text{N/m}^2 \) with \( \pm 1 \text{N/m}^2 \) fluctuations. The direction change at this point is about \( \pm 5 \) degrees. ‘WSS2’ is picked from an impinging area with high OSI on the aneurysm wall; the WSS vector at this point shows a large direction change from -109 to 160 degrees but with extremely small magnitude (0.2 - 0.6 \( \text{N/m}^2 \)).
To make sure that the oscillation is not a numerical artifact, we performed several simulations with different VFRs, smaller $\Delta t$ as well as thorough $p$-refinement tests. These simulations with higher resolutions in space and time confirmed that the observed fluctuations are due to a hydrodynamic instability, and that the numerical solutions converge spectrally fast; see Chapter 3 for more details.

### 7.4 Discussion

A correlation between high WSS and locally elevated pressure in the bifurcation is clearly established from all simulations. Also, high pressure regions inside the aneurysms coincide with the location of the daughter lobule of patient C. It is interesting to notice that the aneurysm in the ICA of patient A is located on the side of the sharp bend as shown in Fig. 7.1 (left). In our studies, we have observed that the sides of turns are high WSS spots when a secondary flow structure is developed. All cases studied for patient D also show that high WSS occurs on the sides of bends at the ICA.

For the cases of patients C and D, the presence of an aneurysm is associated with local high pressure/low WSS locations (4-5 mmHg and 5 $N/m^2$, respectively) surrounded by a band of high WSS (40-60 $N/m^2$) at the distal end of the aneurysm neck. Hence, aneurysms affect the parent blood vessel adversely by creating localized regions of WSS higher than 50 $N/m^2$. The infundibulum also affects adversely the health of the downstream parent vessel by creating high WSS locations (20-30 $N/m^2$ at the distal wall and 40-50 $N/m^2$ at the PCoA bend), as the case AH showed. Once the aneurysm forms at the root of the PCoA in patients C and D, the flow jet impinges onto the aneurysm domes, and high pressure regions with a band of high WSS are formed inside the aneurysms of cases CA and DT. These spots coincide with the locations of the daughter lobule of patient C and the protruding area of the aneurysms of patient D. At the downstream aneurysm of patient D, the impinging flow is not as strong as in the upstream aneurysm on the PCoA bifurcation. However, even a small amount of flow into the aneurysm seems to contribute to vortex generation and high WSS spots (50-60 $N/m^2$) at the neck of the aneurysm.

**Limitations**

The rigid walls for our models can possibly change the magnitude of WSS and pressure and/or the spectrum of velocity/WSS fluctuations. From the reports of Tori et al. [136]
and Oubel et al. [108], we expect that our simulations with rigid walls may overestimate somewhat the WSS magnitude. However, the infundibulae in the PCoA root are similar to lateral aneurysms. As Torii et al. demonstrated that the effect of the deformable walls in a lateral aneurysm case is not as significant as in the terminal aneurysm case, we estimate that the flow structure and WSS distribution do change only negligibly in our case. We have also performed two dimensional simulations with compliant walls and found that the velocity time traces change by less than 10% over a 10-fold change in the elastic modulus of the wall. However, the effect of compliant vessel on the flow instability requires further investigation.

There may be other biomechanical factors that we did not consider in this study; e.g. the blood vessel response to oscillatory WSS may affect the progression of an infundibulum into an aneurysm. However, our present study and findings by others [23, 119, 24, 20, 132, 138, 22, 98] strongly support the thesis that the flow pattern of high WSS/pressure spots in an infundibulum and in an aneurysm play an important role in the progression or rupture of an infundibulum. When flow fluctuates with higher frequencies than the base pulsatile flow, the magnitude and the direction of WSS vectors change dynamically.

In vitro experiments of Davis et al. demonstrated that the unsteadiness of flow plays a more dominant role than the magnitude of WSS [29]. Specifically, they observed that an endothelial cell monolayer under high turbulent shear stress (14 dynes/cm²) for more than 24 hrs develops gaps between cells, which indicates cell retraction and cell loss. Laminar shear stress does not degrade the integrity of the layer except the alignment of the cells along the flow direction. The response of endothelial cells to oscillatory shear flow has been studied and the proinflammatory response are more active under oscillatory flow than steady flow [65]. Hence, the oscillation in the upstream flow as in the patient A due to the presence of an aneurysm may accelerate the degenerative process in the infundibulum. Once an aneurysm grows, the aneurysmal flow tends to be more unstable, and the degradation may accelerate. However, these issues need further experimental investigation.

The higher pressure regions surrounded by a band of high WSS in our simulations seem to be consistent with the rupture locations observed in the aforementioned case reports [83, 27, 28]. Hence, we do not claim that all infundibulae progress into aneurysms. However, our study indicates the strong relationship of the geometric configuration of infundibulae with either rupture or progression into aneurysm observed by many clinicians.
Blood is a non-Newtonian fluid with shear-thinning and yield-stress properties. The effect of shear-thinning property on the flow distribution in large arteries has been studied extensively. Some studies show a dramatic effect [52, 51] while other studies note a small effect during a fraction of the cardiac cycle, specifically near the end of the diastole [74, 110]. Gijsen et al. investigated this discrepancy and pointed out that the higher axial velocity and flow rate increase the shear rate and reduce the shear-thinning effect on the flow. In our simulations, we assumed that the physiological flow rates in the ICA are in the range $200 \sim 400 \text{ml/min}$ with average $275 \text{ml/min}$ based on a previous study [47], which gives the average velocity in the range of $0.26 \sim 0.53 \text{m/s}$ (the diameter of the ICA near the supraclinoid artery in our geometry is less than $4 \text{mm}$ and the characteristic shear rate $8V_a/3r$ [135], where $V_a$ is the average velocity and $r$ is the radius of the blood vessel, ranges $353 \sim 706 \text{s}^{-1}$). When the shear rates are higher than 50 or 100 $\text{s}^{-1}$ [90, 45], blood can be treated as Newtonian with constant viscosity. Hence, in our present study we make sure that the shear rates in our flow conditions are well above 100 $\text{s}^{-1}$. The characteristic shear rates $\sqrt{2 \sum D_{ij} D_{ij}}$, where $D_{ij} = 1/2(\partial u_i / \partial x_j + \partial u_j / \partial x_i), i, j = 1, 2, 3$ are calculated from patient A’s flow field at the end of the distole and are shown in Fig. 7.14 (left). We also compute non-Newtonian viscosity ($\mu$) using three models listed in Table 6.3. The ratio $\mu/\mu_N$ of non-Newtonian viscosity ($\mu$) to Newtonian viscosity ($\mu_N$) used in our simulations is shown in Fig. 7.14 (right). Even inside the aneurysm, the shear rates are above 100 $\text{s}^{-1}$ and the non-Newtonian viscosity ratio ranges from 0.85 to 1.1, which correspond to apparent viscosity of 0.034 $P$ to 0.044 $P$. Hence, we expect that the Newtonian assumption is acceptable in our simulations.

Finally, given the limited number of patients, we cannot make any general conclusion from this study. However, we expect that this study will motivate more interest and systematic studies on the role of infundibulum from the clinical community as well as the research community.

### 7.5 Conclusions

We have performed here the first computational investigation on the effect of a funnel-shaped patient-specific PCoA bifurcation. Using the high-order spectral/hp element method, a series of numerical simulations with patient-specific geometric models and their modifications
revealed that an infundibulum at the PCoA origin may put the neighboring vessels at risk for developing aneurysm by creating high WSS/pressure (40-50 N/m$^2$ and 1 mmHg) spots at the distal infundibulum wall and a spot of low WSS (less than 1 N/m$^2$) with highly oscillatory WSS at the proximal side of the infundibulum. Moreover, an aneurysm at the root of PCoA creates even higher WSS (50-70 N/m$^2$) around the neck of the aneurysm or bifurcation. In the stagnation region in the parent vessel near the aneurysm, the pressure is higher than the neighboring walls by 4-5 mmHg. The flow into the aneurysm creates a high-pressure spot at the aneurysm distal dome. Also, aneurysms may cause hydrodynamic instabilities creating more complicated temporal and spatial variation in terms of WSS magnitude and direction, which is hypothesized to put the blood vessel walls at higher risk of degradation [131, 149, 3, 46]. Either in the infundibulum or in the aneurysms, the impingement locations characterized by higher pressure and surrounding high WSS seem to coincide with the locations of rupture reported in case reports [96, 109, 83, 105, 105] and CFD studies [23, 119, 24, 20, 132, 138, 22, 98]. Hence, the funnel-shaped PCoA bifurcation should be closely monitored by clinicians as has already been suggested in many case reports [28, 129, 73, 27, 96, 109].
Figure 7.1: Patient A (left) and B (right): patient-specific geometric models and zoom-ins of the infundibulum at the root of the PCoA. Bottom row is the close-up view of the circled region in the figures at the top. Colors represent the z-coordinate of the vessel wall for viewing clarity. Left Column: Patient A, infundibular bifurcation at the PCoA root and aneurysm in the cavernous segment. Right Column: Patient B, infundibular bifurcation and aneurysm growing at the junction of the infundibulum and the ICA. The AChA is abnormally large while the diameter of the PCoA at the tip of the infundibulum is small.
Figure 7.2: Geometric models of patient C. Top: aneurysm-removed bifurcation model (left) and aneurysm-laden PCoA bifurcation model (right). Colors represent the $z$-coordinate of the vessel wall. Bottom: Zoom-ins of the circled bifurcation regions in the top row.
Figure 7.3: Geometric models of patient D. Top: Aneurysm-removed (DI), one aneurysm (DO), two aneurysms (DT) models from left to right. Colors represent the $z$-coordinate of the vessel wall for viewing clarity. Bottom: close-up views of circled regions in the top row. The supraclinoid ICA segment is marked with a blue arrow.
Figure 7.4: Patient A: Instantaneous WSS (Top and middle right) and pressure (middle left) distribution at the systolic peak in the supraclinoid segment. Middle right: WSS distribution viewed from the negative z direction. Color and arrows represent WSS magnitude and direction, respectively. Bottom: The colors on the slice represent the velocity normal to the plane. The band of high (low) WSS on the wall is marked with a pink (blue) line and the black arrow indicates the region of high OSI at the proximal end of the infundibulum.
Figure 7.5: Patient A: OSI and average WSS vector distribution at the infundibulum of case AH and the relation between OSI and WSS magnitude. (a) OSI distribution of case AH. The two figures (b,c) on the right are zoom-ins of the circled area. The arrow indicates the viewpoint for the right zoom-ins. (b) OSI distribution at the infundibulum. The circle indicates the region of high OSI in case AH. The red arrow indicates the flow direction in the ICA. (c) Distribution of average WSS magnitude and average WSS vector direction. The circled area is the low WSS region. (d) Plot of average WSS magnitude versus OSI in case AH. Each point represents a point on the vessel wall, i.e., the entire domain. The curve $y = 1/x^{0.5}$ is drawn for better understanding of the distribution of points.
Figure 7.6: Patient A: linear relationship between average WSS and maximum WSS at the vessel walls. Blue and red dots represent the results of case AL (VFR = 250 ml/min) and of case AH (VFR = 300 ml/min), respectively.
Figure 7.7: Patient A: the linear relationship between average WSS and maximum WSS at different locations in case AH. At the aneurysm wall, the points spread out and the slope is higher than the average slope 1.7. Patches labeled as A, B, and C on the left show the regions for sampling maximum and average WSS. The corresponding plots with the same colors and labels (A, B, and C) are shown on the right. Patches A, B, and C correspond to regions of the PCoA infundibulum, of the upstream aneurysm, and of the ophthalmic ICA segment, respectively.
Figure 7.8: Patient B: WSS/pressure distribution and streamlines at the systolic peak of case BA, VFR = 300 ml/min. (a) WSS distribution viewed from the inside of the ICA bend at the PCoA bifurcation. (b) Pressure distribution viewed from the inside of the ICA bend at the PCoA bifurcation. The center line of supraclinoid ICA segment is marked with a blue line. The turn (bend) near the PCoA is marked with a red dotted line and the inside of the turn is marked with a black line. (c) Close-up view of WSS and pressure distribution at the systolic peak, view from the opposite side of the top view, i.e. from the outside of the ICA bend at the PCoA bifurcation. (d) Close-up view of pressure distribution viewed from the opposite side of the top view, i.e. from the outside of the ICA bend at the PCoA bifurcation. (e) Streamlines in the infundibulum and the aneurysm. Viewpoint is the same as that of the top figures.
Figure 7.9: Patient C: Changes in WSS (top) and pressure (bottom) distribution of patient C at the systolic peak. Left column (a,c) is CA model, and the right one (b,d) is CI model. Black arrows point to the area of high local pressure and WSS around the PCoA bifurcation.
Figure 7.10: Patient D: Pressure (top) and WSS (bottom) distribution at the systolic peak: (a,d) DI, (b,d) DO, (c,e) DT. Black arrows point to high local pressure and WSS around the PCoA bifurcation.
Figure 7.11: Patient A: History points and velocity traces at representative points of case AH. The points downstream of the aneurysm on the bend show oscillations during the decelerating systole. (a) locations of several history points (Pt 7, Pt 11, Pt15, and Pt 16) and two points where WSS vectors are recorded (WSS1 and WSS2). (b-e) Velocity time trace at Pt 7, 11, 15, 16. (f-g) Time traces of magnitude and direction of WSS vectors at points WSS1 and WSS2 shown in (a).
Figure 7.12: Patient A: Changes in power spectral density of velocity among history points. The spectrum at the infundibulum decays slower than those of other points. Bottom is the zoom-in of the top figure.
Figure 7.13: History points inside the aneurysm for velocity convergence test. U,V, and W components at A (Pt 1) and B (Pt 10) are plotted on the right and the time-dependent flow rate is also plotted for phase comparison. The red boxes show the time interval where the velocity and WSS errors are measured among different polynomial orders. This particular time interval is chosen because the oscillation starts during the decelerating systole.

Figure 7.14: Patient A: Shear rate calculated from the flow field at the end of the diastole of patient A (left) and ratio of apparent non-Newtonian viscosity ($\mu$) using the Carreau-Yasuda model (right) [25] to Newtonian viscosity ($\mu_N$) used in our simulations. Colors represent the shear rate (left) and the ratio of non-Newtonian viscosity to Newtonian viscosity (right). Iso-surfaces were extracted at the shear rate 100 s^{-1} (left) and the viscosity ratio 1.1 (right).
Chapter 8

Summary

In this thesis, a spectral element method for fluid-structure interaction and flow instability in brain aneurysms are presented with following contributions.

• Fluid-Structure interaction (FSI) simulations in bioflow are very challenging due to the small mass ratio of solid to fluid. FSI is implemented with high-order spectral element method, which couples a fluid solver, NEKTAR, and a solid solver, StressNEKTAR. MPI communication is implemented and all spectral modes on the interface are exchanged between the solid and fluid subdomains. Strong-coupling, i.e. sub-iterations, is implemented to ensure stability and to enforce velocity and pressure continuity. Simulations are stable at small mass ratio of solid and fluid density close to 1. FSI of very thin and flexible tubular structures with small elastic moduli are successfully simulated.

• The computational cost of FSI is very expensive due to a large number of sub-iterations when the density ratio of solid to fluid is small. Fictitious mass and fictitious damping are proposed to improve the stability of FSI and implemented in the StressNEKTAR. It is also shown that fictitious mass and damping larger than actual structural mass increases the number of sub-iterations.

• Blood vessels are surrounded or embedded in various materials and environment not in constant pressure condition. Hence, elements with spring-supports are proposed as a new boundary condition and implemented to model tissues, bones, and tethers surrounding the blood vessel walls. In simulations with straight pipes, stabilizing
effect of the boundary condition is demonstrated.

- Flow instabilities in patient-specific aneurysms are numerically observed. Flows in wide-necked aneurysms tend to become unstable during the decelerating systolic peak and return to pulsatile state at the end of diastole. Large-scale simulations with the Circle of Willis including 30 arteries such as ICA, MAC, ACA, VA, PCA, PCoA, and ACoA, shows that flow can be unstable without aneurysms. Velocity fluctuation agrees with stability analysis of pulsatile flow and experimental data including sound recording or Doppler recording of blood flow in the brain. In order to see the effect of compliant wall on the velocity fluctuations, 2D aneurysmal flow is simulated with compliant walls. The attenuating or amplifying effect of wall compliance is demonstrated to depend on the Young’s modulus of the wall.

- A fast and efficient way to create surface meshes using available tools, Amira and VMTK, is proposed and tested with a large intracranial network. A procedure to extrude inlet/outlet and to split branches using VMTK is tuned with the surface discretization capability of mesh generation software, Gridgen.

- Mesh generation software, Gridgen, can generate only linear elements. To generate isoparametric spectral elements, a visualization algorithm, SPHERIGON, is employed and implemented in NEKTAR. During the preprocessing in NEKTAR, smooth surfaces are reconstructed from vertices and normal vectors at the vertices and spectral elements are projected onto these surfaces. Such spectral elements enhances stability in large-scale simulations by reducing CFL number near the walls. Spectral convergence of solution in a geometry constructed with such projection is confirmed.

- Semi-implicit spectral element method over-resolves a solution in time due to the strict CFL condition which scales as $O(1/P^2)$, when $P$ is the order of spectral elemental polynomial. Hence, a sub-iteration scheme which is stable at larger time step $\Delta t$ and consequently at CFL conditions larger than 1 is investigated. The sub-iteration scheme demonstrates reduction in the divergence error on the boundary, which results in enhancement in stability and accuracy. Stability does not depend on the polynomial order $p$. Compared with fully-implicit scheme, it is more stable and accurate up to larger time step $\Delta t$ of $O(1)$. An implicit solver for the Navier-Stokes equations is
also implemented in the NEKTAR, and high-order temporal accuracy and excellent
stability is obtained although it is conditionally stable.

In aneurysmal flow simulations, there are many mathematical and computational issues
in theory and implementation that need to be addressed and improved. Here I list up
ongoing works and propose future works as long-term projects.

From numerical analysis point of view, the stability of the proposed sub-iteration scheme
and implicit scheme needs to be analyzed. The maximum size of time step in the sub-
iteration scheme seems to be restricted not by CFL condition but by the convergence of
fixed-point iteration and by the range of relaxation parameter. The loss of stability in the
implicit scheme when time extrapolation of nonlinear term is employed needs to be inves-
tigated. The NEKTAR with fully-implicit scheme and StressNEKTAR is not as efficient
as the standard NEKTAR because the preconditioner for both of them is a diagonal pre-
conditioner. Hence, more advanced preconditioners need to be developed or employed and
implemented. The computational efficiency of simulations should be improved for produc-
tion run of FSI code especially at small density ratio cases. The fully-implicit NEKTAR
should be coupled with the StressNEKTAR to allow larger time steps in FSI. From the per-
spective of biophysics applications, the propagation of sound generation should be further
investigated. Validation of FSI simulations is needed for further simulations of compliant
cells.
Appendix A

VMTK

Here we briefly summarize procedures of extrusion, branch splitting, and center line extraction. VMTK(http://www.vmtk.org) has excellent tutorials on how to use the software. Please consult that as well as this section when using the VMTK modules.

Inlet/outlet extrusion

Inlet/outlet extrusions are recommended to create pipe segments which make the imposition of Wommersley boundary conditions easier.

1. Using vmtk surfacewriter and an imported .stl file foo.stl, run the following command:

   vmtk vmtksurfacewriter -ifile foo.stl
   -ofile foo.vtp

   This converts the surface into a vtk polydata file, which you can then use to manipulate.

2. We need open inlets and outlets in order to create flow extensions. If inlets/outlets are capped, run the following command:

   vmtk vmtksurfaceclipper -ifile foo.vtp
   -ofile clippedfoo.vtp

   This will bring up the rendering window. Upon pressing "i" on your keyboard, you will see an interactive box come up which allows you determine how to bound the
region you want to eliminate from the geometry. Press the space bar to proceed with cutting. There is no undo button, so be careful! And the geometry inside of the box is what is eliminated. For the purposes of extensions, clipping orthogonal to the artery is probably best, as is picking the thinnest point (just like we would do in Gridgen).

3. After all clips have been made and all inlets and outlets are open, we can now create flow extensions, which are dependent on the centerlines of the geometry. To create flow extensions, run the following command:

```
vmtksurfacereader -ifile clippedfoo.vtp --pipe vmtkcenterlines
    -seedselector openprofiles
    --pipe vmtkflowextensions
    -adaptivelength 1
    -extensionratio 6
    -normalestimationratio 0.01
    --pipe vmtksurfacewriter -ofile foo_ex.vtp
```

This method will bring up a rendering window a couple of times. Use the enumerations on the inlets and outlets to first specify which are inlets and which are outlets (so that centerlines can be computed), then to specify which of these open profiles you want to extend. The above parameters can change to modify the extensions. For example, ‘adaptivelength’ is a boolean flag that bases the extension on the radius of the tube. ‘extension ratio’ is the ratio of the length of the extension to the radius of the tube being extended. ‘normalestimationratio’ tells VMTK how far down the tube the extension begins. If we are clipping at the exact point where we want our extension to begin, this parameter should be small.

4. Inspect the surface to ensure that the extensions are of good quality. The surface can be inspected by invoking the following command.

```
vmtksurfaceviewer -ifile file.vtp
```

If you want to cap the extensions, run:

```
vmtk vmtksurfacecapper -ifile foo_ex.vtp
    -ofile cappedfoo.vtp
```
Otherwise, save as an stl file and export to gridgen:

```shell
vmtk vmtksurfacewriter -ifile foo_ex.vtp
   -ofile fooSTL.stl
```

**Branch splitting**

Splitting a complicated arterial network into its constituent branches will expedite surface mesh generation in Gridgen.

1. Convert the .stl file to .vtp format.

2. Run the following command:

```shell
vmtk vmtksurfacereader -ifile foo_ex.vtp
   --pipe vmtkcenterlines
   --pipe vmtkbranchextractor
   --pipe vmtkbranchclipper -groupids 0
   -ofile split_geom.vtp
```

This command has to be invoked each time to extract the individual components of the larger geometry you are using. You will be able to specify which branch you want to extract by changing the groupids parameter. Starting with 0 will usually extract the main inlet. Then, each time the module is run, you can change it to `-groupids 1 2` and so on. Sometimes, entering a single number will extract a branch, and sometimes a branch will be defined by two groups, so two numbers will have to be entered. The goal is to keep running the module until you enter a number that brings up an error message that group id does not exist indicating that you have exhausted all possibilities. Group Ids are not repeated, so if you get a geometry that is yielded from specifying `-groupids 1 2` then next time you should run the command with `-groupids 3 4`. Also note that you will be asked to specify the source and target points, which are necessary for computing centerlines. **MAKE SURE YOU SPECIFY THESE POINTS IN THE EXACT SAME ORDER EACH TIME THE MODULE IS RUN!!** Since this module is run repeatedly with the assumption that each branch will be identifiable by the same group ids, and these group ids are based on how source and target points are
specified, it is important to ensure that sources and targets are assigned to the inlets and outlets in the exact same order each time.

Once all branches have been extracted, convert the vtp files to .stls. If you want to increase the surface triangle number, run:

```bash
vmtk vmtksurfacesubdivision -ifile foo.vtp
    -ofile foo_updated.vtp
    -method butterfly
```

**Centerlines**

Extracting centerlines can be a very convenient way of generating 1D models from 3D surface models. For extracting the centerlines of a given geometry,

1. Convert the stl file to vtp.

2. Make sure all inlets and outlets are open. Use vmtksurfaceclipper to open up the inlets and outlets.

3. Once this has been done, run:

```bash
vmtk vmtknetworkextraction -ifile foo.vtp
    -ofile foo_centerlines.vtp
```

This will create a centerlines file, which can be viewed using

```bash
vmtksurfaceviewer -ifile foo_centerlines.vtp
```

In order to view the file as an ascii to get coordinates of center lines, open up in ParaView and convert the file into an ascii text file.
Appendix B

NEKTARfsi

Here I summarize changes in compilation of NEKTAR and new boundary conditions for fluid-structure interaction. More specifically ‘L’ and ‘G’ boundary conditions indicates boundaries where FSI interaction is taking place and springs are attached on the vertices. I describe the procedures on the assumption that compilation and run on the CRAY XT5 machine and the following directory

HYBRID

|-- Veclib
|-- HlibFS
   |--- XT5
   |--- src
|-- Nektar3 dF
   |--- XT5
   |--- src
|-- Nektar3dS
   |--- XT5
   |--- src
|-- Nektar3dSN
   |--- XT5
   |--- src

1. Compile veclib and copy the compiled library to HlibFS/XT5.
2. Compile metis and gs and copy libraries to HlibFS/XT5.

3. cd to HlibFS.

4. Compile HlibFluid library by invoking make ARCH=XT5 FLUID=1 opt.

5. Compile HlibSolid library by invoking make ARCH=XT5 SOLID=1 opt.

6. cd to HYBRID/Nektar3dF

7. make ARCH=XT5 PARALLEL=1 FSI=1 ALE=1 WOMERR=1 opt. Compiling without FSI or ALE will result in Nektar standalone that does not interact or communicate with the solid solver, StressNektar.

8. cd to HYBRID/Nektar3dS for linear StressNEKTAR or HYBRID/Nektar3dSN for non-linear StressNEKTAR.

9. make ARCH=XT5 PARALLEL=1 FSI=1 opt. Compiling without FSI will result in StressNektar standalone that does not interact or communicate with fluid solver, Nektar.

Compilation options (Definitions) defined in the Makefiles under HYBRID/Nektar3dF, HYBRID/Nektar3dS, and HYBRID/Nektar3dS.

- GTYPE - optional for spring supported boundaries
- AITKEN - required for FSI, but optional for standalone Nektar or StressNektar. This enables sub-iteration and relaxation at each time step.
- ALE - required for FSI. This option enables arbitrary Lagrangian-Eulerian description of deformable mesh.

**Gridgen to REA file**

Specify ‘L’ on boundaries where FSI communication, hydrodynamic force transfer from fluid to solid, and velocity and acceleration transfer from solid to fluid, is necessary. Curved faces are supported on ‘L’ type boundaries.

```plaintext
++ do NOT modify the NEXT line +++
1 0 1 interface
```
1 CURVED
A CURVE_TYPE
L TYPE % L type boundary condition
0 LINES
INLINE
0. 0. 0. SI0 % for surface reconstruction

+++ do NOT modify the NEXT line +++
*** CURVED SIDE DATA ***
1 Number of curve types
Recon % Recon type will use SPHERIGON
1 A

Input file for StressNEKTAR

****** PARAMETERS *****
GRIDGEN 3D -> NEKTAR
3 DIMENSIONAL RUN
30 PARAMETERS FOLLOW
10 STRUCTDENSITY % material density
0.0 DADDEDMASS % fictitious mass
5e4 DMODULUS % Young’s modulus
0.3 DPOISSONRATIO % Poisson ratio
0.001 DAMPING_C1 % proportional damping coeff.
0.001 DAMPING_C2 % proportional damping coeff.
0. FICDAMPING % fictitious damping
0 SUPPORT_STIFF % spring constants of attached springs
0.0 STARTIME % time
0.5 DNM_GAMMA % Newmark Scheme
0.25 DNM_BETA % Newmark Scheme
0.5 DTHETA1 % BDF scheme for acceleration
0.5 DTHETA2 % BDF scheme for velocity
4000 IMAXIT % maximum number of sub-iteration
0.3  DINITRELAX  % initial relaxation parameter
1    ITSTART    % time step from which sub-iteration
     % starts
0.0  DLOWER_LIMIT % relaxation parameter
0.98 DUPPER_LIMIT % relaxation parameter
1    MSTRCHK    % Stress field will be saved(dumped)
     % at every IOSTEP
1e-11 DITTOL    % Tolerance for sub-iteration

********** ATTACHED SPRING **********
96 POINTS. Hcode, I,J,H,IEL
-0.0000 1.1050 2.0000 0.0100 % x1 y1 z1 radius1
 1.1050 0.0000 2.0000 0.0100 % x2 y2 z2 radius2
-0.0000 -1.1050 2.0000 0.0100
-1.1050 -0.0000 2.0000 0.0100
-0.2156 1.0838 2.0000 0.0100
-0.4228 1.0209 2.0000 0.0100
...

‘ATTACHED SPRING’ section in the solid REA file contains approximate coordinates where springs are attached. For example, the second line ‘1.1050 0.0000 2.0000 0.0100’ tells the NEKTAR to attach a sping to a vertex located inside a sphere of radius 0.01 centered at (1.105, 0.000, 2.000). At the same time, the boundary should have type ’G’.

Input file for NEKTAR

42 PARAMETERS FOLLOW
0.035849056603774 KINVIS
45 PAVG_STEP % time step to start averaging pressure
    % for a reference
0.05 DSEND_ZERO_FORCES_TIME % time to start sending forces to solid
4000 IMAXIT % maximum number of sub-iteration
1e-5 DITTOL % tolerance for sub-iteration
0.3 DINITRELAX % initial relaxation parameter
1 ITSTART % time step when
% subiteration starts
0. DLOWER_LIMIT % relaxation parameter
0.98 DUPPER_LIMIT % relaxation parameter
...

***** CURVED SIDE DATA *****
1 Number of curve types
Recon % SPHERIGON reconstruction
1 A
19579 Curved sides follow
1 19 A % normal vectors at face 1 of element 19
 0.765692 0.556593 0.574069 % normal x1 x2 x3
 0.631178 0.805881 0.809013 % normal y1 y2 y3
 -0.123816 -0.201891 -0.126263 % normal z1 z2 z3
1 106 A
 -0.997681 -0.931672 -0.990150
 0.064798 0.362101 0.129665
 -0.020826 0.029492 -0.052822
...

Appendix C

Beam Analysis

According to the analysis of Causin et al. in [19], the added mass operator is a mapping from fluid (solid) acceleration at the fluid-structure interface to pressure at the interface. In their study, inviscid and incompressible fluid is considered for analysis. Hence, the interfacial acceleration is the Neumann boundary condition at the wall, and the pressure is obtained from an elliptic equation. The pressure at the wall is just the restriction of the entire solution to the interface. The eigenvalue of the operator is largest when the eigenvector is lowest spatial frequency (lowest mode). This agrees with the analysis of Degroote et al. in [32] which showed that an error mode with a low spatial frequency destabilizes the fixed-point iteration. In structural mechanics, columns under axial compression can be destabilized at critical compression forces, which is called buckling. Constraints are used to avoid such catastrophic failures and the locations of constraint correspond to the nodes of eigenmodes. Supports are also used in beams to change natural frequencies or mode shapes, which may change fundamental frequencies away from resonant frequencies.

The spring supports around the blood vessels are physically more reasonable models for the peripheral boundary conditions and such supports suppress and shift unstable low eigenmodes to more stable high eigenmodes as the constraints for beams are used for better structural stability. The eigenvalues and eigenmodes of beams which has the moment of inertia of corresponding tubes (pipes) are obtained numerically and the effect of attached springs is studied. The material density and Young’s modulus are 1.0 and 1e4 MPa. The cross-sectional area and moment of inertia of the tube are 0.6597 and 0.3645, respectively. The inner and outer radii of the tube are 1.0 and 1.1, respectively. Moment of inertia is
calculated by the formula $I = (R^4_o - R^4_i)\pi/4$. The length of beams are 4, 8, or 16 mm with 80 elements.

For the beam of length 4 mm, a spring is attached in the middle at $x = 2$. Both ends at $x = 0, 4$ are clamped. The spring constants are varied from 0, 1e2, 1e4, to 1e6 to check the effect of spring stiffness on the eigenmodes and eigenvalues. The first four modes are illustrated in Figure C.1. Spring constant 0 corresponds to a beam without any spring support. The eigenvalues are close to analytic eigenvalues.

For the beam of length 8 mm, three springs are attached at $x = 2, 4, 6$. Both ends at $x = 0, 8$ are clamped. The spring constants are varied from 1e2 to 1e4, 1e5, and 1e6 to check the effect of spring stiffness on the eigenmodes and eigenvalues. The first four modes are illustrated in Figures C.2 - C.5. The spring at the center $x = 4$ is fixed at $K_s = 1e2, 1e4, 1e5,$ and $1e6$ while two neighboring springs are set to $r \times K_s$, where $r$ is either 1/4, 1/2, 3/4, or 1. Figures C.2, C.3, C.4, and C.5 correspond to $r = 1/4, 2/4, 3/4,$ and 1, respectively.

For the beam of length 8 mm, we increase the number of spring supports from three to five, which are located in the middle at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. Both ends at $x = 0, 8$ are clamped. The spring constants are varied from 1e2 to 1e4, 1e5, to 1e6 to check the effect of spring stiffness on the eigenmodes and eigenvalues. The first four modes are
Figure C.2: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, $ and $6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two neighboring springs are set to $0.25 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant 1e2, 1e4, 1e5, and 1e6, respectively.

Figure C.3: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, $ and $6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two neighboring springs are set to $0.50 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant 1e2, 1e4, 1e5, and 1e6, respectively.
Figure C.4: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, \text{ and } 6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two adjacent springs are set to $0.75 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, \text{ and } 1e6$, respectively.

Figure C.5: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 2, 4, \text{ and } 6$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and two neighboring springs are set to $1.0 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, \text{ and } 1e6$, respectively.
Figure C.6: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.25 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, and 1e6$, respectively.

illustrated in Figures C.6 - C.9. The spring at the center $x = 4$ is fixed at $K_s = 1e2, 1e4, 1e5, and 1e6$ while four other springs are set to $r \times K_s$, where $r$ is either $1/4, 1/2, 3/4, or 1$. Figures C.6, C.7, C.8, and C.9 correspond to $r = 1/4, 2/4, 3/4, and 1$, respectively.

For the beam of length 16 mm, five springs are attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. Both ends at $x = 0, 16$ are clamped. The spring constants are varied from $1e2, 1e4, to 1e6$ to check the effect of spring stiffness on the eigenmodes and eigenvalues. The first four modes are illustrated in Figures C.10 - C.13. Figures C.10, C.11, C.12, and C.13 correspond to $r = 1/4, 2/4, 3/4, and 1$, respectively.

Figure C.14 shows the changes of eigenvalues as the spring constants increase from 0 to $1e2, 1e3, 1e4, 1e5, and 1e6$. One to five springs are attached to the beams of length 4, 8, and 16 mm.
Figure C.7: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.50 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.

Figure C.8: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.75 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, 1e6$, respectively.
Figure C.9: Eigenmodes of clamped-clamped beam of length 8 mm with springs attached at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $1.0 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2$, $1e4$, $1e5$, and $1e6$, respectively.

Figure C.10: Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.25 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2$, $1e4$, $1e5$, and $1e6$, respectively.
Figure C.11: Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.50 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, \text{ and } 1e6$, respectively.

Figure C.12: Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $0.75 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5, \text{ and } 1e6$, respectively.
Figure C.13: Eigenmodes of clamped-clamped beam of length 16 mm with springs attached at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. The spring constant at the center is set to $K_s = 1e2, 1e4, 1e5, 1e6$ and four other springs are set to $1.0 \times K_s$. (a) 1st mode (b) 2nd mode (c) 3rd mode (d) 4th mode. Solid line, dash line, solid with square symbol, and dash line with triangle correspond to spring constant $1e2, 1e4, 1e5,$ and $1e6$, respectively.
Figure C.14: Eigenvalues ($\lambda_n$) of (a) clamped-clamped beam of length 4 mm with an attached spring of spring constant $K_s = 0$, $1e2$, $1e3$, $1e4$, $1e5$, and $1e6$ at $x = 2$, (b) clamped-clamped beam of length 8 mm with three attached springs of spring constant $K_s = 1e2$, $1e4$, $1e5$, and $1e6$ at $x = 2, 4, 6$, (c) clamped-clamped beam of length 8 mm with five attached springs of spring constant $K_s = 1e2$, $1e4$, $1e5$, and $1e6$ at $x = 1.28, 2.56, 4.0, 5.28, 6.56$. (d) clamped-clamped beam of length 16 mm with five attached springs of spring constant $K_s = 1e2$, $1e4$, $1e5$, and $1e6$ at $x = 2.56, 5.12, 8.00, 10.56, 13.12$. Right plots are zoom-in of the left plots.
Bibliography


