Development of Numerical Tools for Hemodynamics and Fluid Structure Interactions

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Abstract

The aim of this study is to create CFD tools and models capable of simulating pulsatile blood flow in abdominal aortic aneurysm (AAA) and stent graft. It helps to increase the current physiological understanding of rupture risk of AAA and stent graft fixation or migration. Firstly, in order to build a general solver for the AAA modeling with reasonable accuracy, a third/fourth order modified OCI scheme is originally developed for general numerical simulation. The modified OCI scheme has a wider cell Reynolds number limitation. This high order scheme performs well with general rectangular mesh for incompressible fluid. Second, a velocity based finite volume method is originally developed to calculate the stress field for solid in order to capture the transient changes of the blood vessel since the artery is a rubber like material. All one, two and three dimensional classical cases for solid are tested and good results are obtained. The velocity based finite volume method show good potential to calculate the stress field for solid and easy to blend with the finite volume fluid solver. It has been recognized that fluid structure interaction (FSI) is very crucial in biomechanics. In this regard, the velocity based finite volume method is then further developed for FSI application. A well known one dimensional piston problem is studied to understand the feasibility of the fluid structure coupling. The numerical prediction matches the analytical solution very well. The velocity based method introduces less numerical damping compared with a stagger method and a monolithic method. Finally, the work focuses on practical
pulsatile boundary conditions, non-Newtonian blood viscous properties and bifurcating geometry, and provides an overview of the hemodynamic within the AAA model. A modified Womersley inlet and imbalance pressure outlet boundary conditions are originally used in this study. The Womersley inlet boundary represents better approximation for pulsatile flow compared with the parabolic inlet condition. Numerical results are presented providing comparison between different boundary conditions using different viscous models in both 2D and 3D aneurysms. Good agreement between the numerical predictions and the experimental data is achieved for 2D case. 3D stent models with different bifurcation angles are also tested. The Womersley inlet boundary condition improves the existing inlet conditions significantly and it can reduce the Aneurysm neck computation domain. The influence of the non-Newtonian model to the wall shear stress (WSS) and strain-rate is also studied. The non-Newtonian model tends to produce higher WSS at both proximal and distal end of the aneurysm as compared with the Newtonian model (both 2D and 3D cases). The computed strain-rate distribution at the centre of the aneurysm is different between these two models. The influence of imbalance outlet pressure at the iliac arteries to the blood flow is originally investigated. The imbalance outlet pressure boundary conditions affect the computed wall shear stress significantly near the bifurcation point. All the pulsatile Womersley inlet, non-Newtonian viscosity properties and the imbalance pressure outlet need to be considered in blood flow simulation of AAA.
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To my family and my fiancé, Guozhen Wu
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**Nomenclature**

A  area of cross section

$d$ diameter; displacement

d$_i$ displacement component($i=1,2,3$ or $x,y,z$)

D maximum diameter of AAA

E Young’s modulus

I second moment of area

$l$ length of the artery

L length of the bar

$m$ mass

$r$ radius

Re Reynolds number

$p$ pressure

$t$ time

T cardiac cycle

$u$ velocity vector

$u_i$ velocity component($i=1,2,3$ or $x,y,z$)

$\nu$ Poisson ratio

$V$ volume
total force acting on the end of a cantilever beam

coordinate direction x

coordinate direction y

coordinate direction z

Kronecker-delta function

Lame’s first parameter

dynamic viscosity, shear modulus

density

bifurcation angle of AAA

stress tensor

tensile stress

shear stress tensor

at initial time

at the first calculate time

at the second calculate time

back face
B  back point

e  east face

E  east point

f  front face

F  front point

L  at the end of the length

i  iliac location

n  north face

N  north point

neck  at the AAA neck

P  local point

s  south face

S  south point

w  west face

W  west point

Superscripts

0  at the old time

n  at the current time step

n+1  at the next time step

new  at the new time step

old  at the old time step
Chapter 1

Introduction

1.1 Motivation

Abdominal aortic aneurysm (AAA) is a local enlargement of the abdominal aorta exceeding more than 50% of the normal diameter. Abdominal aortic aneurysm, the main subject of this study, commonly occurs below the kidneys. Abdominal aortic aneurysms occur most commonly in individuals between 65 and 75 years old and are more common among men and smokers. The mortality rate of ruptured aneurysms exceeds 65% as reported by a previous study (Harries et al., 2000).

A practical and useful rupture predictor factor of AAA is the maximal aortic diameter. People with a greater maximal aortic diameter have higher rupture risk. Five-year rupture rate for AAAs of less than 4cm maximal diameter is 2%. However, if the maximum aortic diameter is over 7cm, an estimate of five-year rupture rate increases up to 75% (Cavric et al., 2008). The growth mechanism regarding AAA is still not quite certain; however, the pulsatile behaviour of the cardiac cycle has an important influence on the aortic wall.
Large (i.e., those with maximal diameter greater than 5.5 cm) and symptomatic aneurysms are considered for repair by open repair or endovascular repair. Endovascular aneurysm repair (EVAR) involves the use of a stent-graft to exclude aneurysms of the abdominal aorta. A stent graft is a tubular device, which is composed of special fabric supported by a rigid structure, usually metal. The stent-graft is normally fixed by the radial force of the stent which has greater diameter than the normal artery. However, stent-graft migration may occur due to poor fitting into native vessels, and causes late aneurysm rupture, proximal endoleak, graft kinking and graft limb thrombosis. The intraluminal stability of the stent-graft is dependent upon mechanical forces at the proximal and distal fixation sites which are essential related to the blood pressure, blood flow and shape of the aneurysm.

The massive improvements in medical imaging techniques and computing power have already been applied to this problem at a reasonable level. However, current knowledge regarding the initiation, growth and rupture of AAA, forces cause stent migration, and hence the critical parameters and considerations for a numerical study is still lacking. This study mainly focuses on the development of CFD codes and models capable of predicting hemodynamics in the AAA and stent models from patient specific data. The developed methods could be applied to investigate the risk of EVAR and aid the understanding of aneurysm formation, growth and rupture.

1.2 Objective and Strategy

The work concerns the non-Newtonian blood properties and the stresses analysis of a pulsatile flow on the artery wall. The pulsatile nature of the flow and non-Newtonian blood
properties are vital in the modeling of blood flow in the AAA with bifurcation iliac arteries. In large artery with simple geometry (i.e., slight curvature vessel), blood can be assumed as a Newtonian fluid (constant viscosity). However, the geometries of AAA with iliac bifurcation are very complex especially for specific patient. Thus, non-Newtonian models could provide better approximation in this situation. The pulsatile transition condition, the non-Newtonian viscosity model as well as the detailed description of complex bifurcating geometry are crucial and needed to be kept into account in the numerical calculations. Also, FSI plays an important role in modeling the artery wall submerged between blood and intracranial fluid. Computational fluid dynamics (CFD) can only calculate the pressure normal to the artery and the wall shear stress applied to the rigid vessel wall. In order to get a full stresses field of the aorta wall, computational solid mechanics (CSM) need to be applied. To the author’s knowledge, most of the CFD solver use finite volume method while finite element method is more popular in CSM. The combination of these two different methods may lead to numerical unstable if the displacement of the solid domain is large. This study also aims to develop finite volume method to compute both fluid and solid domain in a single solver to reduce the computational cost and capture the instability.

1.3 Outline of the Thesis

This thesis is organized in to 7 chapters. Chapter 2 presents a review regarding the problem of pulsatile blood flow with in the Abdominal Aortic Aneurysm and stent, which covers lots of the experimental and numerical researches reported in the literature, providing
the background of this study.

In order to develop a reasonable solver, a modified operator compact implicit (OCI) scheme is first developed and tested in Chapter 3. One dimensional Burger’s equation and two dimensional shear driven cavity cases are computed and validated with well documented results. Moreover, the accuracy and the reliability of the method are investigated in depth.

In Chapter 4, a velocity based finite volume algorithm for solid is developed. The 1D wave equation is tested first to show the advantages offered as compared to some classical methods. In addition, case of a transient wave propagate in a long steel bar is calculated in both 2D and 3D environment. In order to confirm the capability of the solid solver for 2D and 3D cases, the vibration of a cantilever beam is also investigated. The CFL number effect to the numerical errors is discussed. The temporal accuracy of the velocity based method is also studied in this chapter.

Chapter 5 is concerned with the fluid structure interaction solver for the velocity based method. A one dimensional FSI piston problem is studied and comparisons between the current method and other methods (Blom, 1998) are made. The importance of the geometric conservation law (GCL) for moving mesh (fluid part) and the interaction consistency law (ICL) is also investigated in this chapter.

Numerical simulation of pulsatile non-Newtonian hemodynamic within 2D and 3D AAA models are implemented using finite volume in Chapter 6. An unsteady Womersley expression of inlet velocity distribution based on the pressure wave is developed to obtain more realistic boundary condition. Validation of the numerical prediction is performed in comparison with the experimental results provided by Budwig et al (1993). A fully three
dimensional analysis of velocity and wall shear stress field is presented to have a deep understanding of the hemodynamic. 3D transient analyses of total wall shear stress and drag to the stent graft are discussed in Appendix E. The geometric affect to the total forces acting on the stent is studied in details. Both bifurcated angle and the imbalance iliac diameter affects are investigated. (Appendix E)

Finally, chapter 7 concludes the thesis with a brief summary regarding the method developed. Future work on the current numerical method is also put forward.
Chapter 2

Background

2.1 Introduction

In this chapter, a brief review regarding the prior studies of abdominal aortic aneurysm and the stent reported in the literature is presented. The following sections primarily cover discussions on the statistic analysis, pulsatile analytical analysis, numerical simulations and numerical methods.

2.2 Abdominal Aortic Aneurysms and Stent Graft Migration

Harris et al., (2000) presented a clinical research study about the risk factors of late rupture, stent migration, and death after endovascular repair of aneurysm based on the EUROSTAR (European Collaborators on Stent/graft techniques for aortic aneurysm repair) experience. They reported that 14 patients (out of 2464 patients) were confirmed suffering rupture of aneurysm after endovascular repair and 9 (64.5%) of them were death. A 30-day death rate is below 3% of patients after successful deploying the stent graft. The authors pointed out that the significant risk factors for the stent failure were proximal type I endoleak, midgraft (type III) endoleak, graft migration and postoperative kinking of the endograft. They
also indicated that stent graft migration and postoperative kinking are device-related issues that have significant influence to the rupture of the aneurysm and improvements in the design of stent grafts is required.

Maarit et al., (2005) studied the influence of iliac fixation in prevention of stent graft migration among 173 patients. Their results showed that patients with no stent migration had a greater iliac fixation length than those with migration, and the distal ends of the iliac limbs were closer to the iliac bifurcation than in patients with migration. Among patients with both good iliac fixation and good aortic fixation, no migration occurred. The author also showed that 9% of patients with bad iliac fixation have migration problem while migration were observed in 23% of patients with both bad iliac fixation and aortic fixation. They concluded that iliac fixation along with aortic fixation is an important factor in preventing the migration of stent graft.

Litwinski et al., (2005) studied the role of aortic neck dilation and elongation in the etiology of stent graft migration. They accumulated computed tomographic (CT) images from 308 patients with endovascular AAA repairs using a passive fixation device and found out that 15.6% of the cases have stent graft migration of 5mm or more. The authors reported that 35.4% of the migration patients had a total loss of proximal seal zone. They also concluded that postoperative elongation of the infrarenal aortic neck may create the migration. They suggested that aortic neck dilation beyond oversizing, aortic neck shortening and loss of proximal fixation length are more clinically relevant indicators of proximal stent graft failure.

Sun (2006) investigated the midterm results of transrenal fixation of stent graft with regard to device migration. This study showed that stent graft in all 18 patients undergoing
stent graft fixation moved in the range of 2.6-14.2 mm. The author also pointed out that there is no close relationship between aortic neck angle and stent graft migration.

2.3 Computational Fluid Dynamics for Blood Flow

Shahcheragh et al., (2002) presented a numerical study of pulsatile three-dimensional blood flow in the human aortic arch. The peak Reynolds number in this study is 2500 and the Womersley number is 10. A flat flow velocity profile was used with a pulsatile waveform at the aortic inlet. Results of both flow field and wall shear stress were presented in their paper and their results showed that the velocity profile further downstream is more similar to the shape of the Womersley (Womersley, 1955) solution rather than the parabolic shape. Morris et al., (2005) also studied the 3D numerical simulation of steady and unsteady blood flow based on the real models of human aorta. They pointed out that during maximum deceleration, reverse flow occurs near the inner wall of the artery, while at the maximum acceleration the flow is flattening in the centre of the aorta. They also concluded that steady flow simulations underestimate the recirculation and reversed flow patterns.

Finol and Amon (2001) provided a numerical prediction for 2D pulsatile blood flow in an axisymmetric model of the two-aneurysm abdominal aorta. They assumed the inlet velocity profile is parabolic with unsteady waveform and constant blood viscosity. The authors mainly focused on the WSS distribution and did not show much flow details in this study. Peak WSS occurred in the proximal and distal ends of the aneurysms at peak systole according to their results. They also generalized their study to 3D geometry of human AAAs without iliac bifurcation using a finite element model (Finol and Amon, 2003). Uniform velocity profile
was applied in this research. Flow separation at the proximal neck of the aneurysm occurs during systolic deceleration and single-vortex growth at the midsection and translates further downstream. They noticed that the peak WSS is localized upstream of the proximal end and is 64 times greater than of the normal aorta. Kose et al., (2006) introduced a CFD study of AAAs with patient-specific inflow boundary conditions. They pointed out that the results with patient-specific inlet profiles provide better flow field approximation than with plug-flow inlet profile. However, their method needs to scan MR images for specific patient which is very expensive.

Raghavan and Wedster (1998) investigated the influence of diameter and asymmetry to the mechanical wall stress in AAA using a finite element method. They noticed that the asymmetry of an AAA has an important effect on normal wall stress, and aneurysms with the same diameter may not necessary have the same propensity for rupture. Fillinger et al., (2002) presented an in vivo analysis of mechanical wall stress and AAA rupture risk. Specific AAA models were created based on CT images and finite element method was applied to simulate the wall stresses. Maximum wall stress occurs mostly at the proximal and distal ends of the aneurysm. The authors also concluded that the actual AAA shape and time dependent patient blood pressure waveform may be superior to maximum diameter as the rupture risk factors. They also provided an individual study on wall stress versus diameter in AAA (Fillinger et al., 2002). This study also showed that maximum diameter of AAA is not a key index of AAA rupture risk. In addition, they suggested that a non-invasive analysis of 3-D AAA wall stress is a superior diagnostic parameter for determining AAA rupture risk. Reeps et al., (2010) studied the impact of model assumptions on the computational results in AAA. They pointed
out that the model assumption leads to unforeseeable changes of maximum stresses. They also suggested patient-specific modeling is very important but very expenses in computational resources. Piccinelli et al., (2013) presented a numerical study on lumen boundary displacements in AAA using a 4D-CT technique. In their study, the AAA lumen boundary displacement was tracked for each time frame. New mesh of the lumen boundary displacement (LBD) was generated for new calculation time step. They pointed out that no explicit treatment of turbulence is needed to reproduce the flow impingement location in the AAA according to the measured LBD and simulated WSS. However, their simulation is not a fully coupled fluid structure interaction method.

Kim et al., (2005) presented an analysis of the pulsatile flow and wall stresses in an AAA endovascular stent. The important finding of their study is that the dominating factor is the blood pressure term and that it is strongly depends on the cross-sectional areas of the flow inlet and outlets of their orientation. Guivier-Curien et al., (2009) analysed the pulsatile blood flow behaviour in custom stent grafts. Finite element method is used in their research and sac blood pressure is also considered. They pointed out that the wall shear stress has important contribution to the total drag force on the stent. Molony et al., (2010) presented a migration forces study in patient-specific AAA stent-graft. Magnitude and direction of migration forces are investigated in both idealized and patient-specific model. They showed that the results between idealized and patient-specific model are similar. They also concluded that the anterior-posterior neck angulation of aneurysm has large contribution to the drag force.
2.4 Fluid Structure Interaction

2.4.1 Application of FSI methods in cardiovascular simulation

Scotti et al., (2005) investigated the effects of asymmetry of AAA and wall thickness of artery using a fluid structure interaction computational model. Ideal AAA models with the same maximum diameter were selected and the blood viscosity was assumed constant. The inlet velocity condition is assumed parabolic with time dependent waveform. The authors noticed that the asymmetry effect strongly influence the flow field and contributes to early formation of recirculation regions which yield high velocity gradients at the distal end of AAA. They also pointed out that the decrease of the wall thickness may potential cause the peak wall stress 4 times higher than with the normal uniform thickness. Scotti and Finol (2007) extended their numerical study to patient specific AAA models based on CT images. Both WSS and normal wall stress were calculated finding that WSS level is 4-5 orders magnitude less than the normal stress. Compared to their previous study (Finol and Amon., 2003), predictions of normal stress without FSI may be underestimated up to 25%. The remarkable finding of this study is that the flow-induced pressure gradients in patient-specific AAA geometries have an important impact on the maximum wall stress and its location. In addition, the authors also pointed out that the maximum diameter of AAA does not correlate with the peak wall stress.

Li and Kleinstreuer (2005) studied the blood flow in a stented AAA model using fluid structure interactions. Non-Newtonian fluid model and finite element method were used in their study. The authors mainly focused on the fluid-structure interaction effect to the Endovascular stent graft (EVG) migration. EVG placement may reduce the sac pressure and
wall stress significantly according to their numerical simulation. However, the complex hemodynamics incurs a drag force on the EVG which may cause stent migration. They continued this study in a stented AAA model considering type II endoleaks (Li and Kleinstreuer, 2005). They concluded that the rupture risk of type II endoleaks depends on the inlet branch pressure. Li and Kleinstreuer (2006) also presented an individual study on wall stress and rupture risk of AAA without stent using FSI. According to this study, the neck angle and the iliac bifurcation angle influence the flow field and the stress field substantially. The authors noticed that a large neck angle may cause large irregular vortices in the AAA cavity and influences wall stress remarkably. Takizawa et al., (2012) presented an overview of FSI modeling using various space-time and ALE-VMS techniques. They concluded that the ALE-VMS performs very well in handling patient-specific cardiovascular FSI modeling.

2.4.2 Different FSI methods

Nobile and Vergara (2012) introduced a partitioned algorithm for FSI problems in hemodynamic simulation. The authors considered the Navier-Stokes equations for the fluid in Arbitrary Lagrangian Eulerian form, while the finite elasticity equations for the solid are transferred in Lagrangian form. They applied the Robin-Robin (RR) interface conditions to alleviate the effect of the added mass of the fluid on the structure. A one dimensional FSI piston problem is studied and good agreement of the coupled frequency can be obtained in their study.

Over the last decade immersed-boundary methods (IBMs) have gain attention by many researchers for their capability to solve the FSI problems with large deformation. The IBMs
were first developed by Peskin (1972) to solve flow around the flexible leaflet of a human heart. The advantage of the IBMs is to solve the Navier-Stokes equations on a single rectangular domain where the flexible solids were enabled to be deformed. The IBMs were developed significantly in the past several years. Zhang and Zheng (2007) presented a modified IBMs using the direct-forcing concept in combination with an improved interpolation/extrapolation method. They applied the IBMs to calculate flow over a stationary cylinder, an oscillating cylinder, and a stationary sphere. Their methods improve the stability of the force coupling, simplicity of implementation, and obtain good results with second order accuracy. Devendran and Peskin (2012) introduced an IBM for incompressible viscoelasticity. In their study, Lagrangian coordinates were used to describe elastic forces and Eulerian coordinates were used for the equations of motion and incompressibility condition. The elastic forces are calculated from an energy-based method without using stress tensor. This method can predict good results in both 2D and 3D FSI cases with second order accuracy.

2.5 Conclusions from literature review

2.5.1 Abdominal Aortic Aneurysms and Stent Graft

From the literature reviews, the clinical factor for rupture risk of AAA is the maximum diameter. However, patients with small AAA also face rupture risk of AAA. Wall stress analysis can be used as an alternative choice to predict the rupture risk. The reviews also show that endovascular repair is a powerful surgical method to prevent rupture of AAA. For the current stent graft technique, the stent graft may failure due to type II endoleaks and stent
graft migration (Harris et al., 2000).

Stent graft migration occurs to the patients with bad fixation conditions such as short or no proximal neck and lost of distal fixation (Maarit et al., 2005 and Litwinski et al., 2005). Proximal neck dilation and elongation may also causes lost of proximal fixation of the stent graft. Thus, CFD analysis is required to understand the flow field and wall stresses distribution within the AAAs with and without stent graft.

2.5.2 Computational Researches for Blood Flow in AAA models

Previous studies show that researchers tend to simulate the blood flow, wall stress of the AAA and drag force (WSS and pressure force) to the stent graft separately. The pulsatile nature, the complex geometry of AAA and the blood viscous properties are the most important factors to affect the flow field and WSS distribution.

One main interests of this study are the drag forces on the stent graft and the flow field within the stented region of AAA. Many studies (Kim et al., 2005, Guivier-Curien et al., 2009 and Takizawa et al., 2012) pointed out that the pulsatile behaviour and the stent inlet and outlet locations mainly influence the total drag force which is dominated by the pressure stress. Therefore, the pulsatile nature (inlet and outlet boundary conditions) and the fully 3D geometries need to be considered carefully in this study.

For rupture risk prediction of AAA, the main interest is the peak wall stresses which are more related to the solid nature. Thus, many researches (Raghavan and Wedster 1998, Fillinger et al., 2002 and Piccinelli et al., 2013) focus on wall stress distribution did not concern the fluid flow for the purpose of reducing calculation expense. However, the
unsteady nature of the blood flow is very important to the artery wall. FSI solvers are needed to solve these problems in details.

2.5.3 Fluid Structure Interaction

As discussed in the previous two sections, the pulsatile nature is of great important to the flow field and wall stresses in the AAA, which means that the fluid-structure coupling nature is crucial and the fluid and solid parts can not be treated separately. Researches recently mainly focus on developing FSI simulation tools using a variety of methods i.e. pure finite element (Li and Kleinstreuer 2005), finite volume for fluid plus finite element for solid (Scotti and Finol 2007). These FSI results did show a great improvement compared with those considered the solid part only (without coupling).

Fully coupled FSI methods become more and more popular in resent researches. Immersed boundary methods (Peskin 1972) have gain attention by many researchers in the last decade (Zhang and Zheng 2007, Devendran and Peskin 2012). Good results can be obtained in simple FSI problems using IBMs. However, application of the IBMs in complex FSI problems like AAA modeling is still lacking. Fully coupled FSI solvers that can handle complex cases are desired in the industry.

2.5.4 Overall conclusion

Most of the latest studies considered the AAA geometries reconstructed from real CT images data. However, none of these works consider altogether the flexible artery wall effect, the pulsatile nature, non-Newtonian viscous effect, real geometrical models and stent graft
together due to the high computational expense. Therefore, this study aims at the
development of a coupled FSI solver suitable to calculate the stress field for deformable solid.
Also, the pulsatile boundary effects (inlet and outlet) as well as the non-Newtonian effect of
blood flow (2D and 3D) are studied.
Chapter 3

A modified OCI Scheme for General CFD Use

3.1 Introduction

In practical fluid engineering, currently numerical methods are widely used for a large number of design and development applications. For such circumstances generally higher order schemes are employed to improve the accuracy of the simulation. Central difference scheme (CDS) in the past was a widely used scheme due to its second order accuracy and no diffusion; however, it is also known and widely publicised in the literature that the CDS produces oscillatory results and in some cases instability in problems involving high cell Reynolds numbers. Many higher order schemes including QUICK and the classic OCI suffer from similar problems (J.H. Ferziger and M. Peric., 2002, Ciment et al., 1978).

Ciment et al (1978) in a seminal study introduced a fourth order operator compact implicit method for use with parabolic equations. Their method is easy to use and does not require extra boundary conditions which normally plague higher order schemes. But the classical limitation of a cell Reynolds number is still a huge stumbling block for problems involving especially uniform and non-uniform grids. Subsequently, Berger et al. (1980) developed a generalized OCI scheme that does not have the aforementioned cell Reynolds
number limitation for uniform grids. Turan and VanDoormaal (1988) tested both the classic and the generalized OCI for a 1D case and developed a finite volume based OCI scheme. They also claimed that the classical OCI leads to non-physical oscillations when cell Reynolds number rises above 5.

The present work is aimed at extending the previous classical OCI scheme for use in a general setting and provides suitability for applications involving higher cell Reynolds numbers for non-uniform meshes. This method can then be extended to be used as a main frame for the FSI solver. A one dimensional nonlinear Burger’s equation was chosen to test the present scheme. Further, an in house code for a two dimensional shear driven cavity is developed to assess the scheme credentials for a benchmark application.

### 3.2 Basic Difference Equations and the Modified OCI Method

If one considers the classical one dimensional convection diffusion transport equation for two-point boundary value problems of a general nature, the form is provided in the following operator format:

\[ L(u) = \frac{\partial u}{\partial t} = a(x) \frac{\partial^2 u}{\partial x^2} + b(x) \frac{\partial u}{\partial x} \quad (3-1) \]

The classical operator compact implicit method, which is different from the Padé scheme, (Ciment et al. 1978) suggests the following relationship

\[ Ru(x_i) = QL(u) \quad (3-2) \]

where Q and R are tridiagonal operators which have the form

\[ r^- u_{i-1} + r^0 u_i + r^+ u_{i+1} = q^- L(u)_{i-1} + q^0 L(u)_i + q^+ L(u)_{i+1} \quad (3-3) \]
and for uniform grid spacing $\Delta x$ where

$$q^+ = 6a_i a_{i-1} + \Delta x(5a_{i-1}b_i - 2a_i b_{i-1}) - \Delta x^2b_i b_{i-1}$$  \hspace{1cm} (3-4)$$
$$q^0 = 60a_{i+1}a_{i-1} - 16\Delta x(a_{i+1}b_{i-1} - b_{i+1}a_{i-1}) - 4\Delta x^2b_{i+1}b_{i-1}$$  \hspace{1cm} (3-5)$$
$$q^- = 6a_i a_{i+1} - \Delta x(5a_{i+1}b_i - 2a_i b_{i+1}) - \Delta x^2b_i b_{i+1}$$  \hspace{1cm} (3-6)$$

$$r^+ = \frac{1}{2}\Delta x^2\left[q^+(2a_{i+1} + 3\Delta xb_{i+1}) + q^0(2a_i + \Delta xb_i) + q^-(2a_{i-1} - \Delta xb_{i-1})\right]$$  \hspace{1cm} (3-7)$$
$$r^- = \frac{1}{2}\Delta x^2\left[q^+(2a_{i+1} + \Delta xb_{i+1}) + q^0(2a_i - \Delta xb_i) + q^-(2a_{i-1} - 3\Delta xb_{i-1})\right]$$  \hspace{1cm} (3-8)$$
$$r^0 = -(r^+ + r^-)$$  \hspace{1cm} (3-9)$$

These relationships are fourth order accurate for uniform grid and a set of formula for non-uniform grids is presented in Appendix A claimed as third order accurate. Defining $Re_c = \Delta xb / a$ as the cell Reynolds number, the classical OCI method has the cell Reynolds number limitation (Ciment et al. 1978) of

$$Re_c \leq \sqrt{12} \approx 3.464$$  \hspace{1cm} (3-10)$$

The advantages of the classical OCI scheme are listed as follows:

a) The matrix Q and R are tridiagonal and can be inverted easily.

b) No fictitious points or extra boundary conditions are needed.

c) The source term is easily computed.

d) The method is fourth order accurate in space for uniform meshes and third order accurate for non-uniform meshes.

e) Time dependent methods with OCI are easy to develop and using Crank-Nicolson method one can obtain second order accuracy in time.

The classical one dimensional OCI method considers the operator $(L(u))$ influence on the
local point as well as the upstream and downstream points. However, considering the operator in a more general form one can set up the following relationships between the upstream points’ L(u) value given as:

\[
r^{-u_{i-1}} + r^0 u_i + r^+ u_{i+1} = q^{i-k_+} L(u)_{i-k_-} + q^0 L(u)_i + q^{i+k_+} L(u)_{i+k_+} \tag{3-11}
\]

where

\[
-1 \leq k_-, k_+ \leq 1 \tag{3-12}
\]

These relationship are applicable for non-uniform meshes, if one keeps \( k_-=1 \) but \(-1 < k_+ = k < 0 \) and assuming the flow direction is that of upwind enforcing the use exclusively of the upstream L(u) values. Following the same procedure as in Appendix A, one can obtain the following relationships.

\[
q^0 = -\left[ 12a_{i+k}(k-1)(\Delta x_i^2 - \Delta x_i^2 + \Delta x_\Delta x_+ + 4k\Delta x^2 + 2k\Delta x_\Delta x_+) -2a_{i+k}\Delta x_+(8k^2\Delta x^2 + 4k^2\Delta x_\Delta x_+ -15k^2\Delta x^2 - 3k^2\Delta x_\Delta x_+ + 3k^2\Delta x^2) +6k\Delta x^2 - 6k\Delta x_\Delta x_+ -6k\Delta x^2 + 3\Delta x_\Delta x_+ + 2\Delta x^2) -2b_{i+k}\Delta x_+(\Delta x_- - 2\Delta x_+ - 6k\Delta x_- + 3k\Delta x_+ + 6k^2\Delta x_-) -b_{i+k}\Delta x^2(\Delta x_- + \Delta x_+)(k-1)(\Delta x_+ + 2k\Delta x_- - 3k\Delta x_+ - 4k^2\Delta x_-) \right] 
\]

\[
q^{i-1} = \left[ 12ka_{i+k}(\Delta x_i^2 + \Delta x_i^2 - \Delta x_\Delta x_+ - 2k\Delta x^2 + 2k\Delta x_\Delta x_+) +2a_{i+k}\Delta x_-(4k^3\Delta x^2 - 4k^3\Delta x_\Delta x_+ - 3k^2\Delta x^2 - 3k^2\Delta x_\Delta x_+ + 3k^2\Delta x^2 + 3k^2\Delta x_\Delta x_+ + \Delta x^2) -2k_{i+k}\Delta x_-(\Delta x_- + 3k\Delta x_+ - 3k\Delta x_- - 6k^2\Delta x_-) +kb_{i+k}\Delta x^2(2\Delta x_+ + 3k\Delta x_- - 3k\Delta x_+ - 4k^2\Delta x_-) \right] 
\]

\[
q^{i+k} = \left[ -12a_{i-k}(\Delta x_i^2 - \Delta x_i^2 + \Delta x_\Delta x_-) +2a_{i-k}\Delta x_+(2\Delta x_i^2 - \Delta x_\Delta x_-) -2b_{i-k}\Delta x_-(3\Delta x_- + 2\Delta x_+) +kb_{i-k}\Delta x^2(\Delta x_+ + \Delta x_-) \right] 
\]

\[
r^-\Delta x_-(\Delta x_+ + \Delta x_-) = q^0(2a_0 - \Delta x_+ b_0)
+ q^{i+k}(2a_{i+k} - (2k\Delta x_+ + \Delta x_+)b_{i+k}) + q^{-}(2a_- - (2\Delta x_- + \Delta x_+)b_-)
+r^+\Delta x_+(\Delta x_- + \Delta x_+) = q^0(2a_0 + \Delta x_- b_0) + q^{i+k}(2a_{i+k} - (2k-1)\Delta x_- b_{i+k}) + q^{-}(2a_- - \Delta x_- b_-)
\]

\[
r^0 = -(r^+ + r^-) \tag{3-12 to 3-17}
\]
The present study originally considers $k=1/2$ implying the use of the mid values between the local point and the upstream neighbor point. In this case, the relationship of equations 3-12 to 3-17 can be further simplified as shown in Appendix A. For a practical nonlinear problem, the choice of $k_-, k_+$ depends on the upstream flow direction. The operator values depend on the upstream value which is the originality of this modification. This modified OCI scheme is tested for both one-dimensional and two-dimensional nonlinear problems.

### 3.3 Numerical experiment for one-dimensional problem

In this section are reported the results of the performance of the modified OCI scheme for both one-dimensional linear and non-linear problems. Since the classical OCI method is unconditionally stable under the cell Reynolds number limitation (Ciment et al. 1978), it can be seen from Appendix A; the same attributes are applicable to the modified OCI as the classical OCI once appropriate choices are adopted for $k_-, k_+$. The extended OCI is also unconditionally stable. The tests as will shown reveal that the modified upwind OCI has a wider cell Reynolds number applicability.

#### 3.3.1 One-dimensional linear parabolic equations with boundary value

The first numerical benchmark considers the solution of a one-dimensional linear parabolic partial differential equation with constant coefficients but varying source as given:

$$L(u) = \mu \frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} = Ax + B$$

(3-18)

with $0 \leq x \leq 1$, $u(0) = 0$ and $u(1) = 1$
When \( A=B=0 \), the analytical solution of the above equations is

\[
\frac{\exp\left(-\frac{x}{\mu}\right) - 1}{\exp\left(-\frac{1}{\mu}\right) - 1}
\]

This particular study is designed to test the accuracy and stability of different schemes under consideration for different cell Reynolds numbers. Results are shown in Table 3-1 and in Appendix B (Figure B1-B6). For certain high cell Reynolds numbers, central difference scheme, QUICK scheme and classical OCI schemes may lead to results displaying non-physical oscillations. Turan and VanDoormaal (1988) presented a detailed study involving CI (Compact Implicit) and OCI schemes in a widely publicised NASA effort; they obtained the same oscillatory behaviour at high cell Reynolds numbers.

As shown in Table 3-1 and Fig. 3-1, when the cell Reynolds number is not high, say \( \text{Re}_c \leq 1.0 \), the classical OCI scheme performs the best among all the tested schemes. The modified OCI displays a fairly good accuracy level compared with the third order QUICK scheme, but is generally less accurate than the classical OCI at low cell Reynolds numbers. This is primarily due to the additional upwind effect in the truncation error. It is clear from the results (Table 3-1, Fig 3-1, Fig. B3 and B6) that the modified OCI does not have a cell Reynolds number limitation. Further, for cell Reynolds numbers above 2.0, the upwind OCI scheme performs even better as compared with the classical one.

For practical problems, in the solution domain where variables display rapid changes, the solution behaviour is all the more critical. Therefore, in practical problems a non-uniform grid is usually preferred for solution economy. Fig. 3-2, Table 3-2 and Appendix B show the results for different non-uniform meshes for the classical and upwind OCI schemes. The
mesh is designed to be finer near the down stream boundary where the values change significantly. Different grid expansion ratios are considered.

The results show that when the maximum cell Reynolds number of the non-uniform grid remains less than 2.0, the classical OCI scheme still provides as good a resolution as that of the uniform grid. However, when the maximum cell Reynolds number is relatively high, the predictive performance of the classical OCI degrades rapidly. The upwind OCI still shows a very good accuracy level even at very high cell Reynolds numbers. Fig. B6 also shows that the upwind OCI can display acceptable behaviour even at high cell Reynolds numbers. The above conclusions are valid only for the linear problem attempted; however, most physical problems such as flow are distinctly non-linear; therefore non-linear benchmark assessments have to be carried to display the suitability of the OCI scheme.

![Graph showing error vs. Cell Reynolds Number](image)

Fig. 3-1 Comparison of linear constant coefficient parabolic equation among different schemes (uniform mesh).
<table>
<thead>
<tr>
<th>Scheme</th>
<th>Number of point</th>
<th>$\mu$ (cell Reynolds number)</th>
<th>Max Error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Central difference</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>-0.1 (1.0)</td>
<td>0.345*10-1</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>-0.05 (0.2)</td>
<td>0.123*10-2</td>
<td></td>
</tr>
<tr>
<td>400</td>
<td>-0.05 (0.05)</td>
<td>0.767*10-4</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>-0.05 (2.0)</td>
<td>0.135</td>
<td></td>
</tr>
<tr>
<td>10</td>
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<tr>
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<td>-0.01 (10.0)</td>
<td>Oscillation</td>
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<td></td>
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<td>Oscillation</td>
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Table 3-1 Comparison of linear constant coefficient parabolic equation among different schemes (uniform mesh).

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<tr>
<th>Scheme</th>
<th>Number of point</th>
<th>Expand Ratio</th>
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<th>Max Error</th>
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<td></td>
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<td>1.2</td>
<td>-0.05 (3.34)</td>
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</tr>
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<td><strong>Modified Upwind OCI</strong></td>
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<td></td>
<td></td>
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<td>-0.1 (1.48)</td>
<td>0.335*10-2</td>
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<tr>
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<td>1.2</td>
<td>-0.1 (1.99)</td>
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</tr>
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<td>-0.1 (3.60)</td>
<td>0.382*10-2</td>
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<tr>
<td>40</td>
<td>1.1</td>
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<td>0.173*10-3</td>
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<td>-0.002 (46.481)</td>
<td>0.105*10-1</td>
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</tr>
<tr>
<td>40</td>
<td>1.3</td>
<td>-0.002 (115.4)</td>
<td>0.136*10-2</td>
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</tr>
</tbody>
</table>

Table 3-2 Comparison of linear constant coefficient parabolic equation between the classic and the modified upwind OCI schemes (non-uniform mesh).
3.3.2 Non-linear Burgers equation

Ciment et al (1978) chose the one dimensional Burgers equation to test the classical OCI scheme as an prototype nonlinear problem. The present work adopts the same problem in order to reveal predictive performance differences between the classical and the current upwind OCI schemes. If one consider the one dimensional nonlinear equation given as:

$$L(u) = \frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial x^2} + (a - u) \frac{\partial u}{\partial x}$$  \hspace{1cm} (3-20)

The exact steady state solution for the above equation is given as

$$u(x) = a(a - \tanh(ax/2\mu))$$  \hspace{1cm} (3-21)

This solution exhibits large gradients near $x=0$, and a steep shock wave forms occurs
when $\mu \to 0$. A number of problems with constant $a=1/2$ employing various values of $\mu$ were solved in the domain $x \in [-5, 5]$. Exact values of $u(x)$ are applied at the boundaries and the initial guesses used are:

$$u(x, 0) = \begin{cases} 
1, & -5 < x < 0, \\
0.5, & x = 0, \\
0, & 0 < x < 5.
\end{cases}$$

(5-22)

A second order Crank-Nicholson method is used to solve this time dependant problem. A similar iteration strategy as that of Ciment et al (1978) is adopted to approximate the nonlinear term. Since the comparison between the classical OCI scheme and second order schemes has already been carried out by Ciment et al (1978), the current study focuses on the classical and the modified OCI only. A wider range of $\mu$ values is tested and the results are shown in Fig. 3-3, 3-4, Table 3-3, 3-4 and Appendix B. The time step for all the cases shown in the tables is taken to be $\Delta t = 0.5$.

For a uniform mesh (Fig. B7), the classical OCI scheme can provide for more accurate results when the maximum cell Reynolds number is at a reasonably low level, say $|Re_{c_{\text{max}}}| < 2$. As the cell Reynolds number increases (Fig. B8), the results of modified OCI scheme remain at reasonable accuracy levels, but the accuracy of the classical OCI scheme degrades unless additional grid nodes are employed. Further, Ciment et al (1978) pointed out that for $|Re_{c_{\text{max}}}| > 2.55$ physical steady state solutions cannot be obtained for the classical OCI scheme. The modified OCI can still provide physical steady state solutions for high cell Reynolds number, implying suitability for a wider range of cell Reynolds numbers.

In order to obtain a rational assessment regarding the scheme performance for practical problems, the use of non-uniform grids is in most cases imposed, i.e., in a channel flow, the
mesh near the wall is finer than near the centre line. Additional focus is naturally placed in specific solution zones where the variable values change rapidly leading to adoption of finer grids in such regions. Thus tests were also carried out for a problem involving a non-uniform grid finer at x=0 where the velocity gradient is highest.

It is worth emphasizing that even at the low cell Reynolds numbers, simply increasing the mesh density provides for an oscillatory solution for the classical OCI scheme unless PE<1 (Fig. B11). The reason for this is attributable to the large time step employed. The solution can be smoothed by decreasing the time step to a ‘satisfactory level’; however, the upwind scheme does not suffer from such deficiencies. The classical OCI fails to provide physical results at the high cell Reynolds number even when the mesh is refined; implying the maximum cell Reynolds number limits the stability of the classical OCI scheme. The modified OCI still performs in a satisfactory manner at the very high cell Reynolds number. Further, refining the mesh near the centre, while at the same time keeping the same number of nodes overall, improves the accuracy significantly (Fig. B10 and B12).

An accepted rationale associated with the use of higher order schemes involves substantial reductions in memory and computing resources while at the same retaining acceptable accuracy. OCI schemes have many advantages in that regard and they are relatively easy to design and implement. The classical OCI has a certain cell Reynolds number limitation, implying for large Reynolds problems grid refinement for acceptable engineering/physical results of sufficient accuracy. The modified OCI scheme adopted in this study also has a wide cell Reynolds number applicability. In addition, it is recommended for use with non-uniform meshes. In the next section, the OCI scheme will be applied to a
realistic numerical benchmark problem.

Fig. 3-3 Comparison of steady state solution of Burgers equation (second order Crank-Nicolson) between the classic and the modified OCI schemes for uniform mesh.

Fig. 3-4 Comparison of steady state solution of Burgers equation (second order Crank-Nicolson) between the classic and the modified OCI schemes for non-uniform mesh.
<table>
<thead>
<tr>
<th>Scheme</th>
<th>Number of point</th>
<th>$\mu$</th>
<th>Max Cell Reynolds Number</th>
<th>Max Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Classic OCI</td>
<td>10</td>
<td>0.5</td>
<td>1.00</td>
<td>0.132*10^{-2}</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.5</td>
<td>0.50</td>
<td>0.796*10^{-4}</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.5</td>
<td>0.20</td>
<td>0.206*10^{-5}</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>0.5</td>
<td>0.10</td>
<td>0.127*10^{-6}</td>
</tr>
<tr>
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<td>2.00</td>
<td>0.189*10^{-1}</td>
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<td>0.25</td>
<td>1.00</td>
<td>0.126*10^{-2}</td>
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<tr>
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<td>0.25</td>
<td>0.40</td>
<td>0.315*10^{-4}</td>
</tr>
<tr>
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<td>0.25</td>
<td>0.20</td>
<td>0.195*10^{-5}</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>0.125</td>
<td>4.00</td>
<td>Diverge</td>
</tr>
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<td>0.125</td>
<td>2.00</td>
<td>0.187*10^{-1}</td>
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<td>0.311*10^{-4}</td>
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<td>0.570*10^{-1}</td>
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<tr>
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<td>Diverge</td>
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Table 3-3 Comparison of steady state solution of Burgers equation (second order Crank-Nicolson) between the classic and the upwind OCI schemes for uniform mesh.
<table>
<thead>
<tr>
<th>Scheme</th>
<th>Number of point</th>
<th>$\mu$</th>
<th>Expand Ratio</th>
<th>Max Cell Reynolds Number</th>
<th>Max Error</th>
</tr>
</thead>
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<td>1.2</td>
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Table 3-4 Comparison of steady state solution of Burgers equation (second order Crank-Nicolson) between the classic and the upwind OCI schemes for non-uniform mesh.
3.4 Numerical Results for Two-dimensional Shear Driven Cavity

3.4.1 Governing equations and numerical methods

The two-dimensional incompressible Navier-Stokes equations are now tackled. In addition to the continuity equation,

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{3-23}
\]

the momentum equations is given as:

\[
\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\partial P}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} \tag{3-24}
\]

\[
\rho \frac{\partial v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} = -\frac{\partial P}{\partial y} + \mu \frac{\partial^2 v}{\partial x^2} + \mu \frac{\partial^2 v}{\partial y^2} \tag{3-25}
\]

The momentum equations can also be expressed as

\[
\frac{\partial u}{\partial t} = \left( \frac{\mu \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x}}{\rho} \right) + \left( \frac{\mu \frac{\partial^2 u}{\partial y^2} - v \frac{\partial u}{\partial y}}{\rho} \right) - \frac{\partial p}{\partial x} = L(u) \tag{3-26}
\]

\[
\frac{\partial v}{\partial t} = \left( \frac{\mu \frac{\partial^2 v}{\partial x^2} - u \frac{\partial v}{\partial x}}{\rho} \right) + \left( \frac{\mu \frac{\partial^2 v}{\partial y^2} - v \frac{\partial v}{\partial y}}{\rho} \right) - \frac{\partial p}{\partial y} = L(v) \tag{3-27}
\]

No slip wall condition is used and the fluid is assumed as Newtonian with constant viscosity.

The geometry and boundary conditions are shown in Fig. 3-5.
Since both the classical and the modified OCI schemes lead to equation (3-2), employing a Crank-Nicolson time discretization and following Ciment et al’s (1978) procedure, the momentum equation can be expressed as:

$$\begin{align*}
(I - \frac{\Delta t}{2}(Q_{x}^{n+1})^{-1}R_{x}^{n+1}) & (I - \frac{\Delta t}{2}(Q_{y}^{n+1})^{-1}R_{y}^{n+1}) u_{i,j}^{n+1} \\
\frac{A_{i,j}^{n+1}}{B_{i,j}^{n+1}} & \\
= (I + \frac{\Delta t}{2}(Q_{x}^{n})^{-1}R_{x}^{n}) (I - \frac{\Delta t}{2}(Q_{y}^{n})^{-1}R_{y}^{n}) u_{i,j}^{n} + \frac{\Delta t}{2} Su_{i,j}^{n+1}
\end{align*}$$

(3-28a)

or

$$\begin{align*}
\left(\frac{Q_{x}^{n+1} - \frac{\Delta t}{2} R_{x}^{n+1}}{A_{i,j}^{n+1}}\right) & \left(\frac{Q_{y}^{n+1} - \frac{\Delta t}{2} R_{y}^{n+1}}{B_{i,j}^{n+1}}\right) u_{i,j}^{n+1} \\
= Q_{x}^{n+1}Q_{y}^{n+1}\left[ (I + \frac{\Delta t}{2}(Q_{x}^{n})^{-1}R_{x}^{n}) (I - \frac{\Delta t}{2}(Q_{y}^{n})^{-1}R_{y}^{n}) u_{i,j}^{n} + \frac{\Delta t}{2} Su_{i,j}^{n+1} \right]
\end{align*}$$

(3-28b)

where the index n+1 refers the values at the new time step and Su refers the source term which contains the pressure gradient and boundary conditions. Since both Q and R are
tridiagonal matrices and the source matrix $S_{i,j}^n$ is easy to compute, equation (3-28) is easily solved by applying the TDMA solver. In order to couple the velocity and the pressure field, the classical SIMPLE algorithm is used. The system of Equations (3-28) for momentum has the form:

$$A_p^{n+1}u_{ip}^{n+1} + \sum_l A_p^{n+1}u_{ij}^{n+1} = Q_p^{n+1} - \left( \frac{\partial p^{n+1}}{\partial x_i} \right)_p$$

(3-29)

SIMPLE type algorithms suggest that the correct velocity can be expressed as

$$u_{ip}^m = u_{ip}^{m*} + u_{ip}^m - \frac{1}{A_p^m} \left( \frac{\partial p^{m-1}}{\partial x_i} \right)_p$$

(3-30)

Due to the nature of the OCI scheme, the collocated grid arrangement is a good choice to adopt. It is mentioned in the literature that a collocated arrangement of values leads to oscillating pressure field, due to the severing of the link between the pressure and control volume interface velocity. Rhie and Chow (1983) proposed a collocated grid arrangement for velocity components that reintroduces in an ad hoc manner the link between the velocities and the local pressure field. The collocated grid arrangement is shown as Fig. 3-6 and the interpolated cell face velocity is thus expressed as:

$$u_e^* = \left[ (u_e^*) - \frac{1}{A_p^m} \left( \frac{\partial p^{m-1}}{\partial x} \right)_e - \frac{\partial p^{m-1}}{\partial x} \right]$$

(3-31)

Fig. 3-6 The collocated grid arrangement.
The velocities are required to satisfy the continuity equation, so one substitutes the correct velocities into the mass flux expression to obtain:

$$\left( \rho u_e^m - \rho u_w^m \right) \Delta y + \left( \rho v_n^m - \rho v_s^m \right) \Delta x = 0 \tag{3-32}$$

Substituting equation (3-30) and (3-31) into (3-32), one eventually derives the final pressure-correction equation as:

$$B_P \dot{p}_P + \sum_{l} B_l \dot{p}_l = -\Delta \dot{m}, \quad l = E, W, N, S \tag{3-33}$$

An ADI (Alternating Direction Implicit) solver is used to solve the pressure-correction equation. The pressure term is discretized using a central difference method. Although the problem to be solved for refers to a steady state flow field, the specific code developed is designed to handle a transient flow field. Steady solution is obtained by running in a time marching manner until the solution reaches steady state. All the velocities and pressure fields are initialized as zero at the first time step.

### 3.4.2 Results and Discussion

In the present study, different meshes are employed to solve for the shear driven cavity flow at Re=10 and 100. In order to compare the accuracy of the results, benchmark accurate solutions (for Re=100) calculated by Ghia et al (1982) are used. For Re=10, results produced by FLUENT with 300×300 grid are considered as an accurate solution.

Fig. 3-7 and 3-8 illustrate the comparison of centre line velocity profile between the two OCI schemes and the FLUENT solution at Re=10. It can be seen that both the classical and the upwind OCI schemes can predict the flow field with a reasonable accuracy. The classical OCI scheme tends to display relatively more accurate results for this problem. The
comparison also shows that use of OCI schemes require fewer grid points for comparable accuracy. Fig. 3-9 also shows that using a non-uniform mesh can further improve the accuracy levels. Fig. 3-10 shows the comparison at Re=100 with a uniform mesh. Since the overall Reynolds number is now increased to 100, using a $16 \times 16$ grid for the classical OCI leads to non-physical oscillations. Thus the grids for the classical OCI scheme have to be refined to $32 \times 32$ and $50 \times 50$. It can be observed that the modified OCI scheme produces larger error as compared with the classic OCI scheme. This may be caused by the additional artificial diffusivity generated by Equation 3-31. The results further show that the classical OCI predicts quite accurate solutions when accompanied by suitable meshes. As discussed in the previous section, the modified OCI scheme does not in general require a very fine grid for comparable accuracy. With $16 \times 16$ nodes, the modified OCI scheme can still predict reasonable results.

The above discussion shows that the OCI scheme can be applied to solve practical flow field problems. The classical OCI scheme has a comparably high accuracy level when the cell Reynolds number is small. The modified OCI scheme can handle the high cell Reynolds number condition with a reasonable level of computational resources. In engineering applications, different schemes are blended together to obtain stable solutions. Hybrid scheme is one of the most widely used schemes blending a first order Upwind Difference Scheme (UDS) and the second order CDS. Since the classical OCI and the modified OCI have the same matrix format, it is possible to further blend them together for increased accuracy in a future study.
Fig. 3-7 Comparison of centre line U velocity profile with uniform mesh at Reynolds number 10.

Fig. 3-8 Comparison of centre line V velocity profile with uniform mesh at Reynolds number 10.
Fig. 3-9 Comparison of centre line U velocity profile at Reynolds number 10.

Fig. 3-10 Comparison of centre line U velocity profile with uniform mesh at Reynolds number 100.
3.5 Concluding Remark

OCI schemes are easy to implement and use and display fourth order accuracy (uniform mesh). They can also be adopted to solve practical engineering flow problems. The classical OCI scheme displays a very good accuracy level among the various schemes tried at a low cell Reynolds number. At high cell Reynolds numbers when the classical OCI fails to predict acceptable results, the modified upwind OCI scheme tends to perform better. The modified OCI has a wider range of cell Reynolds number applicability compared with the classical OCI scheme. Both the classical and upwind OCI schemes are suitable for use with non-uniform grids and they are shown to be third order accurate.

In the future, the current in-house code developed for the OCI scheme would be accessed for more demanding and challenging engineering cases. Since the classical OCI scheme has a very good accuracy level at low cell Reynolds number and the modified upwind OCI is stable for high cell Reynolds numbers, the authors would also consider appropriate strategies for blending the classical OCI with the upwind OCI for improved accuracy in a general CFD setting.

However, both the classic and the current OCI schemes can only be applied with rectangular mesh in the current format. The OCI family numeric schemes can be applied to get more accurate results for simple geometry using rectangular grid. This method need to be further developed to solve the complicate FSI problem. Since many IBMs developed recently are based on the rectangular grid (Zhang and Zheng 2007, Devendran and Peskin 2012), the family of OCI scheme shows good potential to join with the immerse boundary methods. In
the next chapter, a velocity based finite volume method for solid elasticity is developed and tested.
Chapter 4

Velocity Based Finite Volume Method for Solid Elasticity

4.1 Introduction

The artery wall is strongly interacting with the blood flow. The blood vessel is a rubber like material and should be considered as a deformable solid. In order to analyse the full stresses field on the artery wall, the artery considered as a deformable solid should also be computed. Most CSM solvers are based on finite element methods, while the CFD users prefer finite volume methods. The author would introduce a velocity based finite volume method for solid in this chapter. The ultimate goal for this method is to couple both fluid and solid in a single solver. An in house code (1D, 2D and 3D) written in Fortran 95 is developed to solve the solid velocity, displacement and stresses fields.

4.2 Numerical Method

Since both fluid and solid are continua and their behavior can be described by the similar continuity and momentum equations. The only difference between these two media is the constitutive laws. The equations of fluid are solved for velocity and pressure while those of
solid are solved for displacement. The constitutive law for solids in this study assumes a linear elastic (Hookean) solid. Assuming the material is isotropic, which means the elastic constants are the same for any Cartesian coordinates, then the generalized Hooke’s law can be described as

\[ \sigma = 2\mu \varepsilon + \lambda \text{tr}(\varepsilon)I \]  
\[ \text{or } \sigma = \mu \mathbf{D} + \mu (\nabla \mathbf{D})^\top + \lambda \text{tr}(\nabla \mathbf{D}) \]

where

\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial d_i}{\partial x_j} + \frac{\partial d_j}{\partial x_i} \right) \]

where \( \varepsilon \) is the deformation tensor, \( \mu \) and \( \lambda \) are Lame’s coefficients, which can be expressed by the Young’s modulus of elasticity and Poisson’s ratio \( \nu \).

\[ \mu = \frac{\gamma}{2(1+\nu)} \]

\[ \lambda = \frac{\nu \gamma}{(1+\nu)(1-\nu)} \quad \text{for plain stress} \]

\[ \lambda = \frac{\nu \gamma}{(1+\nu)(1-2\nu)} \quad \text{for plain strain and 3D} \]

### 4.2.1 Velocity based formulations for solid

The stagger type algorithms for FSI coupling solve the fluid and solid with different solvers, therefore, additional procedures and iterations are needed to transfer and couple the force balance at the interface. Christina (2004) suggested an idea to solve the solid with velocity based equations. The idea of this chapter is using velocity based equations to solve
the momentum equations for solid similar as fluid. Thus, both fluid and solid can be solved simultaneously. Since the solid equations are based on displacement, the displacement can be expressed from the integral of the velocity from \( t_0 \) to \( t \)

\[
D(t) = \int_{t_0}^{t} U dt = \int_{t_0}^{t} \frac{1}{2} \Delta t U dt + \int_{t_0}^{t} \frac{1}{2} \Delta t U dt
\]

(4-7)

where \( \Delta t \) is the time difference between two time step and \( \Delta t = t - t_0 \). From equation 6-7, the displacement at \( t \) can be approximated as

\[
D^n = D^0 + \frac{\Delta t}{2} (U^n + U^0)
\]

(4-8)

where \( U^0 \) is the velocity calculated from the previous time step and \( U^n \) is the velocity at the present time step. Thus, the stress tensor for the solid equation can be described as

\[
\sigma = \Sigma^+ + \frac{\Delta t}{2} [\mu \nabla U + \mu (\nabla U)^T + \lambda \text{tr}(\nabla U)I]
\]

(4-9)

and

\[
\Sigma^+ = \Sigma + \frac{\Delta t}{2} [\mu \nabla U^0 + \mu (\nabla U^0)^T + \lambda \text{tr}(\nabla U^0)I]
\]

(4-10)

where \( \Sigma \) is the accumulated stress from the previous time steps.

\[
\Sigma = \mu \nabla D^0 + \mu (\nabla D^0)^T + \lambda \text{tr}(\nabla D^0)I
\]

(4-11)

Then the momentum equation for solid over time interval \( \Delta t \) can be written as

\[
\frac{\partial \rho U}{\partial t} = \frac{\Delta t}{2} [\nabla \cdot (\mu \nabla U) + \nabla \cdot [\mu (\nabla U)^T] + \lambda \nabla \cdot [\text{tr}(\nabla U)I]] + \nabla \cdot \Sigma^+
\]

(4-12)

The only differences between this solid momentum equation and fluid momentum equation are the coefficients \( \frac{\Delta t}{2} \mu \) for solid (instead of the viscosity \( \eta \) in fluid) and the additional source term \( \nabla \cdot \Sigma^+ \) for solid (instead of \( \nabla p \) in fluid) (Christina 2004). Therefore, the FSI nature can be simulated using a single set of equations and a single grid domain. The solution procedure for both fluid and solid can be shown in Fig.4-1.
4.2.2 Velocity based equation for 1D wave equation

In order to test the performance of the velocity based equation for solid, the 1D wave equation is tested. The velocity based idea can be transferred to the 1D wave equation using equations 4-7 and 4-8 as

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 d_{\text{old}}}{\partial x^2} + \Delta t \frac{\partial^2 u^*}{\partial x^2} \tag{4-13}
\]

where the average velocity between two time step is

\[
u^* = \frac{1}{2} (u_{\text{old}} + u_{\text{new}}) \tag{4-14}
\]

then

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 d_{\text{old}}}{\partial x^2} + \frac{\Delta t}{2} \left( \frac{\partial^2 u_{\text{old}}}{\partial x^2} + \frac{\partial^2 u_{\text{new}}}{\partial x^2} \right) \tag{4-15}
\]
with boundary conditions and initial conditions as

\[ u(x = 0, t) = 0 \quad \text{and} \quad u(x = L, t) = 0 \]

\[ u(x, t = 0) = 0 \quad \text{and} \quad d(x, t = 0) = d_0 \sin \pi x \] (4-16)

The velocity based 1D wave equation can be derived implicitly at node \( i \) as

\[
\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{d_{i+1}^n - 2d_i^n + d_{i-1}^n}{\Delta x^2} + \frac{\Delta t}{2} \left( \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} \right) 
\] (4-17)

This is actually a tri-diagonal matrix system and can be solved by the TDMA (Tridiagonal Matrix Algorithm) solver.

### 4.2.3 Finite volume discretization for 2D and 3D solid and solution algorithm

The finite volume discretization is based on the integral form of the equation 4-12 over the control volume. The convection term on the left hand side can be neglect for solid. Using the Gauss’ theorem, equation 4-12 can be express as

\[
\int_{V_r} \frac{\partial \rho U}{\partial t} dV = \frac{\Delta t}{2} \int_{\partial V_r} \nabla \cdot (\rho \dot{U}) + \nabla \cdot [\mu(\nabla U)^T] + \lambda \nabla \cdot [\text{tr}(\nabla U)] I + \int_{\partial V_r} \nabla \cdot \Sigma^+ 
\] (4-18)

and

\[
\int_{\partial V_r} \nabla \cdot \Sigma^+ = \frac{\Delta t}{2} \int_{\partial V_r} \rho \dot{\nabla} U^0 + \mu(\nabla U^0)^T + \lambda \text{tr}(\nabla U^0) I + \int_{\partial V_r} \rho \dot{\nabla} D^0 + \mu(\nabla D^0)^T + \lambda \text{tr}(\nabla D^0) I 
\] (4-19)

The above equation will be discretized in a segregated manner, where each component of the displacement vector is solved separately and the inter-component coupling is treated as source explicitly. This approach will lead to well-structured diagonally dominant sparse matrices which can be solved easily.

The discretization of the velocity based method is now presented on a term-by-term basis. First, the temporal derivative is calculated using only one old-time level of velocity components:
\[
\frac{\partial u}{\partial t} = \frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t}
\]  
(4-20)

This form of discretization is second-order accurate in time, since the discretization of the right hand side is based on the time level between the current time step and the new time step.

The volume integrals are evaluated using the mid-point rule:

\[
\int_{V_{p}} \frac{\partial u}{\partial t} dV = \frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} V_{p}
\]  
(4-21)

where \( V_{p} \) is the volume of the CV. The surface integrals in equation 4-18 are the sum of integrals over the cell faces in the CV. The discretization of the Div-Grad term is calculated as:

\[
\int_{V_{p}} \nabla \cdot (\mu \nabla u) dV = \int_{S} dS \cdot (\nabla u) = \sum_{\text{face}} u_{\text{face}} s \cdot (\nabla u)_{\text{face}}
\]  
(4-22)

The summation term can be expressed as

\[
s \cdot (\nabla u)_{\text{face}} = \left| s \right| \frac{u_{\mu} - u_{p}}{d_{\mu}}
\]  
(4-23)

where \( s \) is the face vector and \( d_{\mu} = \overrightarrow{PN} \), and assuming they are parallel.

For the explicit gradients can be calculated using very simple interpolated relation:

\[
(\nabla u)_{\text{face}} = f_{i} (\nabla u)_{p} + (1 - f_{i}) (\nabla u)_{N}
\]  
(4-24)

where \( f_{i} \) is the interpolation coefficient and this term is now calculated from the current values of \( u \).

The fully discretizations for 2D and 3D equations in Cartesian and Cylindrical coordinates are presented in Appendix C. The finite volume method leads to a set of linear equations as

\[
A_{w} u_{w} + A_{s} u_{s} + A_{p} u_{p} + A_{n} u_{n} + A_{e} u_{e} = \text{source}_{i} \quad \text{(for 2D case)}
\]  
(4-25)

or
\begin{align*}
W_{w}u_{w} + A_{s}u_{s} + A_{n}u_{n} + A_{p}u_{p} + A_{e}u_{e} + A_{w}u_{w} + A_{e}u_{e} &= source_{i} \quad \text{(for 3D case)} \quad (4-26)
\end{align*}

or in matrix form

\begin{align*}
[A][u] &= [source] \quad (4-27)
\end{align*}

where W, E, S, N, B, F and P denote the west, east, south, north, back, front and local point of the control volume. The strong implicit procedure (SIP) method is used to solve the 2D linear equations and the ADI method is applied to solve the 3D linear equations. The residual of the solution will be converged to $10^{-6}$. The velocity based method for solid provides a set of linear equations similar to those for fluid, this method can be further developed to solve the fluid structure interaction process. The structure of the code will also be presented in Appendix D.

### 4.2.4 Boundary conditions

The Boundary conditions for solid, either constant or time varying, can be listed of the following types:

(i) fixed displacement or velocity: fixed value at the boundary(constant or time varying)
\begin{align*}
d_{f} &= \text{constant} \quad \text{or} \quad u_{f} = \text{constant} \quad (4-28)
\end{align*}

(ii) fixed pressure or traction and free surfaces(zero traction): the surface force at the boundary $f_{b}$ can be directly applied to the control volume.
\begin{align*}
f_{b} &= |s_{b}|t - s_{b}p \quad (4-29)
\end{align*}

where t and p is the specified traction and pressure.
(iii) planes of symmetry at face $f$.

\[
\left( \frac{\partial d}{\partial x} \right)_f = 0 \quad \text{or} \quad \left( \frac{\partial u}{\partial x} \right)_f = 0
\]  

(4-30)

4.3 Numerical Experiment of 1D Wave Problem

First, the 1D wave equation is validated to test the feasibility and accuracy of the velocity based method for solid. If the initial condition of the 1D wave problem is set to be

\[
d(x,t=0) = \sin(\pi x)
\]  

(4-31) then the analytical solution is only determined by the wave speed $c$.

\[
d(x,t) = \sin(\pi x)\cos(c\pi t)
\]  

(4-32)

In order to test the performance of the numerical method, results calculated by the classic two time steps implicit scheme and the three time steps implicit scheme are used for comparison. Central difference scheme is used for space discretization for the wave equation 4-13.

The computational domain of the 1D wave problem is discretized with 101 nodes. The comparisons of the 1D wave displacement three different schemes and the exact solution at different CFL numbers are shown in Fig. 4-2 and 4-3. At CFL=1 all temporal schemes predict the frequency and amplitude correctly. The results also indicate that the velocity based scheme shows less damping ($7.508 \times 10^{-6}$) than both two time steps implicit scheme($1.199 \times 10^{-4}$) and three time steps implicit scheme($3.002 \times 10^{-5}$). It is clear that the left hand side (LHS) of the velocity based method is a first order derivative and the LHS of the displacement wave equation is a second order derivative. The discretization of the second
order time derivative need two old time steps while the first order derivative only require one old time step. As the CFL number is increased, the velocity based scheme performs better than the other two methods. At CFL=10, the prediction using the velocity based algorithm simulate more accurate frequency of the 1D wave problem. It is apparent that this method shows less temporal numerical damping and less deviation for solid.

The first numerical experiment shows that the velocity based algorithm is suitable to be a solid solver. Moreover, it is more accurate compared with two classic temporal discretization methods.

![1D Wave](image)

**Fig. 4-2** Displacement at the middle point (x=L/2) of the spring (1D wave equation) at CFL=1; With red: exact solution, brown: two time steps implicit, blue: three time steps implicit and black: velocity based.
Fig. 4-3 Displacement at the middle point (x=L/2) of the spring (1D wave equation) at CFL=10; With red: exact solution, brown: two time steps implicit, blue: three time steps implicit and black: velocity based.

### 4.4 Numerical Experiment of 2D and 3D solid

In order to test the velocity based method is also suitable for 2D and 3D cases, we shall now present two example transient calculations. Jasak and Weller(2000) calculated a transient wave propagation in a bar using displacement based finite volume method. This is taken as the first example. The second example is to calculate the vibration and displacement of a cantilever beam.
4.4.1 Stress wave travels in a bar

Consider a thin steel bar with 10m long and 1m wide, the bar is assumed under plane stress condition (for 2D cases). The initial condition is $d=0$ and $u=0$ everywhere. A fixed displacement of 1mm is applied at the left end of the bar; the right end is fixed. This will cause the propagation of the stress wave (pressure wave) through the bar at the speed of sound $C$:

$$C = \sqrt{\frac{E}{\rho}} = \sqrt{\frac{2 \times 10^5}{7854}} = 5046.2 \text{ m/s}$$

(4-33)

The stress wave start at the left end, when the wave reaches the other end of the bar it will reflect and travel backwards. The Poisson’s effect which causes a secondary effect of the transverse waves is also visible. Plane stress assumption is taken for the 2D cases. The mesh consists of 100x10 control volumes (CVs) and the residual of the solution will be converged to $10^{-7}$ for each time step. Fig. 4-4, 4-5 and 4-6 present the distribution of the x-displacement $d_x$, the normal stresses $\sigma_{xx}$, $\sigma_{yy}$ and the shear stress $\tau_{xy}$ for CFL=0.5 at $t=0.0015$s, $t=0.0045$s and $t=0.01$s respectively. The current results are in line with Jasak and Weller’s (2000) stresses simulation using the finite volume displacement method. This shows that the finite volume method also has good potential to calculate the solid mechanics.
Fig. 4-4 Transition wave distribution of (a) $d_x$ contour, (b) $\sigma_{xx}$ contour, (c) $\sigma_{yy}$ contour and (d) $\tau_{xy}$ contour for CFL=0.5 at t=0.0015s.
Fig. 4-5 Transition wave distribution of (a) $d_x$ contour, (b) $\sigma_{xx}$ contour, (c) $\sigma_{yy}$ contour and (d) $\tau_{xy}$ contour for CFL=0.5 at $t=0.0045s$. 


The transient wave can be clearly seen from the three figures. The stress wave travels from the left to right at the beginning, when it reaches the right boundary it reflects and
travels back to the left hand side. The wave will reflect again and again when it reaches the two sides boundaries. The calculation will also be done on different time step sizes of $5 \times 10^5$, $10^5$ and $10^6$s, giving different CFL numbers 2.5, 0.5 and 0.05. The time history of $d_x$ and $\sigma_{xx}$ at the middle point of the bar is shown in Fig. 4-7. The wave should reach the mid point in exactly 0.991 ms, this is clearly seen in the time trace.

Fig. 4-7 Time history of $d_x$ and $\sigma_{xx}$ at the middle point of the bar in different CFL numbers.
Fig. 4-8 shows the displacement time history comparison between the current velocity based method and Jasak and Weller’s method (CFL=0.5). The results show good agreement with the Jasak and Weller’s (2000) results. The simulation also indicates that the current method is of second order accuracy in time as compared with Jasak and Weller’s calculation.

The figures (Fig.4-7) show that the transverse wave reduces much quickly at high CFL number. This is due to numerical diffusion introduced by the large time step size. However, the low CFL number results over and underestimate the stress at the steep gradient. This is cause by the numerical dispersion when the gradient of the value is steep.

![Time history comparison of $d_x$ at the middle point of the bar at CFL=0.5.](image)

A 3D steel bar which is 10m long, 1m wide and 1m depth with $100 \times 10 \times 10$ CVs is also calculated. Figure 4-9 and 4-10 show the mid x-y plane contour of displacement and stresses.
at $t=0.0015s$ and $t=0.0045s$. The results are similar as the 2D simulations.

Fig. 4-9 Mid-plane transition wave distribution of (a) $d_x$ contour, (b) $\sigma_{xx}$ contour, (c) $\tau_{xy}$ contour for CFL=0.5 at $t=0.0015s$.

Fig. 4-10 Mid-plane transition wave distribution of (a) $d_x$ contour, (b) $\sigma_{xx}$ contour, (c) $\tau_{xy}$ contour for CFL=0.5 at $t=0.0045s$. 
Fig. 4-11 also shows a 3D displacement and stresses contour presentation at t=0.01s. The secondary transverse wave due to the Poisson’s effect is clearer in the 3D case. Transition values of $d_x$ and $\sigma_{xx}$ at the middle point of the bar is also shown in Fig. 4-12. The wave also propagates to the mid point in 0.991 ms and the CFL effect is similar as the 2D cases. It should be pointed out that the numerical dispersion at low CFL number is more significant in 3D cases and it leads to unrealistic stress oscillation. Therefore, it is very important to select suitable CFL number to get good results.

![3D transition wave distribution](image)

Fig. 4-11 3D transition wave distribution of (a) $d_x$ Iso-surface slices, (b) $\sigma_{xx}$ contour slices, (c) $\tau_{xy}$ contour slices for CFL=0.5 at t=0.01s.
Fig. 4-12 Time history of $d_x$ and $\sigma_{xx}$ at the middle point of the bar in different CFL numbers for 3D cases.
In order to understand the mesh and time step size effect on the accuracy of the results, history of $d_x$ at the mid point is present with different mesh and time steps in Fig. 4-13 (2D cases) and 4-14 (3D cases).

![Graphs showing time history of $d_x$ at the middle point of the bar in different CFL numbers for 2D cases.](image)

Fig. 4-13 Time history of $d_x$ at the middle point of the bar in different CFL numbers for 2D cases.
Fig. 4-14 Time history of $d_4$ at the middle point of the bar in different CFL numbers for 3D cases.
It can be observed that higher CFL number leads to low numerical dispersion but high numerical dissipation. While low CFL number causes high numerical dispersion and less numerical dissipation. It is clear that the CFL number affect the accurate level significantly. The results also indicate that CFL number should be carefully selected \((0.5 \leq \text{CFL} \leq 1)\) to get the best results.

### 4.4.2 Bending and vibration of a cantilever beam

Since the above tests do not apply any force loading at the boundary, a cantilever beam with a shear loading at one end is also tested in this section. The steel bar is originally set to be 10m long, 1m width with the left end fix and the other end has \(-10^7\) N shear loading at y direction (Fig. 4-15). The analytical solution of the deflection \(d_{\text{end}}\) at the free end is

\[
d_{\text{end}} = \frac{WL^3}{3EI}
\]  

where \(W\) is the shear loading, \(L\) is the length of the beam, \(E\) is the Young’s modulus and \(I\) is the second moment of area about the neutral axis for a beam. The calculated end deflection show good agreement with the analytical solution (Fig. 4-16).

![Fig. 4-15 Cantilevered Beam with an end load.](image-url)
Plane stress condition is assumed as previous section for 2D cases. Fig. 4-17 shows the displacement and stresses distribution at steady state when the shear loading is applied at the end of the beam. Since this method mainly focuses on the transient solver for solid which can also calculate fluid flow, the stresses fields for the steady state of the cantilever beam are not discussed more details here.
According to the beam theory, the first natural frequency \( \omega_f \) of a beam is calculated by

\[
\omega_f = 1.875^2 \sqrt{\frac{EI}{\rho AL^3}}
\]  

(4-35)
where $A$ is the area of the cross section. The steady state result calculated before is then considered as the initial condition, the vibration of the beam can be simulated by freeing the shear loading. The time history of the free end deflection for different geometry and materials is shown in Fig. 4-18. It is clear that the results capture the vibration frequency very well.

Fig. 4-18 Free end displacement vibration of different cases.
Table 4-1 presents the geometry details, parameters and vibration frequency for different cases. The velocity based unsteady solver works very well and it can compute the vibration frequency of different range correctly. It can be concluded that the current method is suitable to simulate linear elastic solid.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)2D &amp;3D</th>
<th>(e)</th>
<th>(f)</th>
<th>(g)</th>
<th>(h)</th>
<th>(i)</th>
</tr>
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<tr>
<td>Length(m)</td>
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<td>8</td>
<td>10</td>
<td>10</td>
<td>0.1</td>
<td>0.1</td>
<td>0.12</td>
<td>0.09</td>
<td></td>
</tr>
<tr>
<td>Width(m)</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>0.01</td>
<td>0.01</td>
<td>0.006</td>
<td>0.003</td>
<td></td>
</tr>
<tr>
<td>Density(kg/m³)</td>
<td>7854</td>
<td>7854</td>
<td>7854</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>Young’s modulus(Pa)</td>
<td>2×10¹¹</td>
<td>2×10¹¹</td>
<td>2×10¹¹</td>
<td>4×10⁸</td>
<td>4×10⁹</td>
<td>1×10⁸</td>
<td>1×10⁸</td>
<td>1×10⁸</td>
<td></td>
</tr>
<tr>
<td>Analytical frequency(Hz)</td>
<td>32.6</td>
<td>12.73</td>
<td>8.15</td>
<td>0.51</td>
<td>3.23</td>
<td>323.04</td>
<td>51.07</td>
<td>21.28</td>
<td>18.9</td>
</tr>
<tr>
<td>Computed frequency(Hz)</td>
<td>32.1</td>
<td>12.72</td>
<td>8.16</td>
<td>0.51</td>
<td>3.23</td>
<td>323.84</td>
<td>51.10</td>
<td>21.42</td>
<td>19.2</td>
</tr>
</tbody>
</table>

Table 4-1 Geometries details, parameters and vibration frequency for different cases.

In order to test the 3D solver for this example, case d is selected to calculate under 3D environment. The depth of the beam is considered to be 1m which is the same as the width.

The free end displacement vibration can be observed in Fig. 4-19.

![Free end displacement vibration of 3D case (d).](image)
The calculated vibration frequency for case d is 0.51Hz which is the same as the analytical solution. Fig. 4-20 and 4-21 also presents the 2D and 3D stress distribution within the geometry. Both figures are displayed when the beam is blend at the maximum deflection. The Poisson’s effect can be observed clearly with in these figures.

Fig. 4-20 Mid-plane (x-y plane) displacement and stresses distribution of (a) $d_y$ contour, (b) $\sigma_{xx}$ contour, (c) $\sigma_{yy}$ contour, (d) $\sigma_{zz}$ contour and (e) $\tau_{xy}$ contour for case d.
Fig. 4-21 3D displacement and stresses distribution of (a) Iso-surface of $d_y$, (b) $\sigma_{xx}$ contour, (c) $\sigma_{yy}$ contour and (d) $\tau_{xy}$ contour for case d.
4.5 Conclusion

The authors would like to point out that this method provides both displacement and velocity field of the solid. The transit solutions match previous research (Jasak and Weller, 2000) and analytical solution in a very good level. The velocity based method can also predict a very detailed stresses field for solid. The current method does not consider the elemental value conservation for solid. If the deformation of the solid is not large, the results without consideration of the volume conservation of solid are almost the same. However, when the deformation of solid is large, the conservation of volume should be considered. Hence, more details development of this method need to be considered in the future. The final aim of this method is to couple the fluid and solid together with less information loss at the interface. Therefore, the next Chapter mainly focuses on a simple 1D FSI problem to understand the potential of the algorithm.
Chapter 5

Fluid Structure Interaction Using Velocity Based Finite Volume Algorithm in Simple Piston Problem

5.1 Introduction

In chapter 4 already tested the velocity based method for solid has been thoroughly validated. Since the main purpose of the velocity based method is to couple both solid and fluid in a single solver, this chapter will focus on the application to a 1D piston problem of the velocity based method. The accuracy of the method and the important factor of the FSI coupling are also studied.

5.2 Numerical Experiment of 1D Piston FSI Problem

5.2.1 1D FSI Problem

The FSI piston problem consists of a pipe with length L filled with compressible fluid with density of $\rho$ as the fluid part. The left-hand side of the pipe is closed at a wall and on the right hand side a moving piston is placed. This piston with mass m is connected to a linear spring with spring constant k (Fig. 5-1). The piston is considered as the structure part.
Therefore, this is a typical one dimensional FSI problem.

\[ \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho u \\ u \otimes \rho u + p \\ u(\rho E + p) \end{pmatrix} = 0 \] (5-1)

where \( \rho, u, p \) and \( E \) denote the density, velocity, pressure and total energy, respectively. Assuming all these values vary only in \( x \) direction, the one-dimensional Euler equations can be expressed as

\[ \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ u \rho u + p \\ u(\rho E + p) \end{pmatrix} = 0 \] (5-2)

The equations are closed by the state equation for a perfect gas

\[ p = (\gamma - 1)\rho \left( E - \frac{1}{2}u^2 \right) \] (5-3)

where \( \gamma \) is the ratio of the specific heats.

If the variables are described as a mean value and an added perturbation, and the
following notations are introduced

\[ \rho = \bar{\rho} + \rho' \]
\[ u = \bar{u} + u' \]
\[ p = \bar{p} + p' \] (5-4)

where \( \bar{\rho} \), \( \bar{u} \) and \( \bar{p} \) are the mean values and \( \rho' \), \( u' \) and \( p' \) are the perturbation values.

In order to linearise the equations, the following approximations are made

\[ \bar{\rho} \gg \rho' \]
\[ c_s \gg u' \]
\[ \bar{p} \gg p' \] (5-5)

where \( c_s \) is the isentropic speed of sound defined by

\[ c_s^2 = \left. \frac{\partial p}{\partial \rho} \right|_s \] (5-6)

The linearised energy equation at isentropic conditions is always satisfied and the acoustic fluid equations can be expressed as

\[ \frac{\partial \rho'}{\partial t} + \bar{\rho} \frac{\partial u'}{\partial x} = 0 \quad \text{and} \quad \bar{\rho} \frac{\partial u'}{\partial t} + c_s^2 \frac{\partial \rho'}{\partial x} = 0 \] (5-7)

or

\[ \frac{\partial p'}{\partial t} + \bar{\rho} c_s^2 \frac{\partial u'}{\partial x} = 0 \quad \text{and} \quad \bar{\rho} \frac{\partial u'}{\partial t} + \frac{\partial p'}{\partial x} = 0 \] (5-8)

These can also be expressed as

\[ \frac{\partial^2 p'}{\partial t^2} - c_s^2 \frac{\partial^2 p'}{\partial x^2} = 0 \] (5-9)

The movement of the piston can be described by the undamped equation of motion for a one degree of freedom model.
\[
m \frac{\partial^2 d}{\partial t^2} + kd = f \quad \text{and} \quad f = (p_L - p_a)A
\]

(5-10)

Where \( k \) is the spring coefficient, \( d \) is the piston displacement, \( p_a \) is the ambient pressure, \( p_L \) is the pressure at \( x=L \) and \( A \) is the area of the piston.

The eigenfrequency of the coupled piston problem \( \omega \) can be calculated from

\[
\kappa L \tan \kappa L = \frac{\rho L}{m \left(1 - \frac{\omega^2}{\omega_n^2} \right)}
\]

(5-11)

where \( \kappa = \omega/c_s \) is the wave number and \( \omega_n = \sqrt{k/m} \) is the frequency of the piston without coupling. The eigenfrequency also shows if the surface force coupling is strong or not.

### 5.2.3 Discretization of the 1D Piston Problem

First, the acoustic equation is considered. If the domain of the fluid is divided into \( N \) nodes and \( N-1 \) cells, the system of the acoustic equation can be discretized by the finite volume method. The temporal Crank-Nicolson method shows the discretized equation for node \( i \) can be expressed as

\[
\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{1}{2\rho} \left( \frac{p_{i+1/2}^n - p_{i-1/2}^n}{\Delta x} + \frac{p_{i+1/2}^{n+1} - p_{i-1/2}^{n+1}}{\Delta x} \right)
\]

(5-12)

and

\[
\frac{p_i^{n+1} - p_i^n}{\Delta t} = -\frac{\rho c_s^2}{2} \left( \frac{u_{i+1/2}^n - u_{i-1/2}^n}{\Delta x} + \frac{u_{i+1/2}^{n+1} - u_{i-1/2}^{n+1}}{\Delta x} \right)
\]

(5-13)

The non-linear Euler equations are considered next since these are simplified version of the Navier-Stokes equations. One difficult task for FSI problem is that the computation
domain of fluid will change every time step. Although the displacement of the piston is small in this case, the Euler equations are formulated on a general deformable coordinate system to test the feasibility of this algorithm. Arbitrary Lagrangian Eulerian (ALE) method is considered for moving mesh. In order to satisfy the geometric conservation law (GCL) for the moving mesh of fluid, the 1D Euler equations on a moving domain can be shown to read

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \rho (u-w) \\ (u-w) \rho u + p \\ (u-w) \rho E + up \end{bmatrix} = 0$$

(5-14)

or

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho (u-w)}{\partial x} = 0$$

(5-15)

$$\frac{\partial u}{\partial t} + (u-w) \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0$$

(5-16)

$$\frac{\partial E}{\partial t} + (u-w) \frac{\partial E}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0$$

(5-17)

where \( w \) is the grid velocity which defined by \( w_i = (x_i^{n+1} - x_i^n) / \Delta t \). These equations are closed by the state equation for a perfect gas. These equations can be discretized using Crank-Nicolson method as

$$\frac{\rho_i^{n+1} \Delta x^{n+1} - \rho_i^n \Delta x^n}{\Delta t} = \frac{\Delta x^{n+1}}{2} \left( \frac{\rho(u-w)_{j+1/2}^n - [\rho(u-w)]_{j-1/2}^n}{\Delta x^n} + \frac{[\rho(u-w)]_{j+1/2}^{n+1} - [\rho(u-w)]_{j-1/2}^{n+1}}{\Delta x_{n+1}} \right)$$

(5-18a)

$$\frac{u_i^{n+1} \Delta x^{n+1} - u_i^n \Delta x^n}{\Delta t} = \frac{\Delta x^{n+1}}{2} \left( \frac{(u_i^n - w_i)(u_{i+1/2}^n - u_{i-1/2}^n)}{\Delta x^n} + \frac{(u_i^{n+1} - w_i)(u_{i+1/2}^{n+1} - u_{i-1/2}^{n+1})}{\Delta x^{n+1}} \right) - \frac{\Delta x^{n+1}}{\rho_i^{n+1}} \left( p_{i+1/2}^{n+1} - p_{i-1/2}^{n+1} \right)$$

(5-18b)
\[
\frac{E_{i}^{n+1} \Delta x_{i}^{n+1} - E_{i}^{n} \Delta x_{i}^{n}}{\Delta t} = \frac{\Delta x_{i}^{n+1}}{2} \left[ \left( u_{i}^{n} - w_{i} \right) \left( E_{i+1/2}^{n} - E_{i-1/2}^{n} \right) \right] + \left( u_{i}^{n+1} - w_{i} \right) \left( E_{i+1/2}^{*} - E_{i-1/2}^{*} \right) \left( \frac{\Delta x_{i}^{n+1}}{\rho_{i}^{n+1}} \right) \left( up_{i+1/2}^{n+1} - up_{i-1/2}^{n+1} \right)
\]

(5-18c)

The velocity based method for the time integration of the piston is discussed in this section.

The motion equation of the piston for one degree of freedom can be expressed by velocity as

\[
\frac{\partial u}{\partial t} = -\frac{k}{m} \left[ d_{o} + \frac{1}{2} \left( u_{L}^{n} + u_{L}^{n+1} \right) \right] + A \left[ p_{L} - p_{s} \right]
\]

(5-19)

Since the integration of the surface pressure need to be consistent with the velocity discretization.

The average pressure has to be applied.

\[
p_{L} = \left( p_{L}^{n} + p_{L}^{n+1} \right)
\]

(5-20)

Thus equation 5-19 can be discretized as

\[
\frac{u_{L}^{n+1} - u_{L}^{n}}{\Delta t} = -\frac{k}{m} \left[ d_{o} + \frac{\Delta t}{2} \left( u_{L}^{n} + u_{L}^{n+1} \right) \right] + \frac{A}{2} \left[ \left( p_{L}^{*} + p_{L}^{n+1} \right) - p_{s} \right]
\]

(5-21)

The fluid, structure and the moving mesh need to be strongly coupled together to simulate a correct result. For the velocity based method, the solid equations do not have to be solved separately, so that both fluid and solid are solved simultaneously. For common finite volume method, the Navier-Stokes equations are solved in an iterative manner. Thus, the velocity based algorithm is also inverted iteratively.

The coupling procedure starts initial the values of the new time step with the previous values. Then the acoustic or the Euler equations for moving mesh are solved iteratively. Notice that, the piston velocity \( u_{L} \) is calculated simultaneously with the momentum equation. At the end of each iteration, the mesh is updated with the piston displacement \( d_{L} \).
\[ d_{L}^{n+1} = d_{L}^{n} + \frac{\Delta t}{2} (u_{L}^{n} + u_{L}^{n+1}) \quad \text{and} \quad x_{i}^{n+1} = \frac{i-1}{N-1} d_{L}^{n+1}. \]

The iteration stops until the error of solution is converge to $10^{-6}$. Also, the boundary conditions at both ends of the pipe need to be considered. For velocity, no slip wall condition is assumed, which means $u=0$ at $x=0$ and $u=u_{L}$ at $x=L$. The other values at the boundary are linearly extrapolated from the interior. The extrapolated variables at both ends are calculated by

\[
\phi_{0} = 2\phi_{1} - \phi_{2} \quad \text{and} \quad \phi_{N+1} = 2\phi_{N} - \phi_{N-1}.
\]

This method avoids additional values updating at the interface between fluid and solid. Since the momentum equation for solid is now with the same value (velocity) of the fluid equation, the force couplings at the interface do not have to be integrated again. This can reduce unnecessary integration loss for the surface force.

### 5.2.4 Results and Validation

The values of the parameters for this problem are first set to be the same as Blom’s (1998) research. The eigenfrequency can be calculated from equation 5-11. Two more cases are studied to test the performance of the numerical method. The parameters chosen in this paper are listed in Table 5-1. The eigenfrequency of the compressible fluid in a pipe is calculated by considering the mass of the piston as infinity. The value is $\omega_{f} = 1030.96 \text{rad/s}$ . The solution of eigenfrequency for the first case is 341.6 rad/s. The frequencies of the piston, the fluid and the coupling various quite a large ranges, which indicates a strong coupling nature of this FSI problem. Two more cases are tested to show the accuracy of the velocity based algorithm.
<table>
<thead>
<tr>
<th>Parameters</th>
<th>Cases</th>
<th>a (Blom’s)</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L (m)$</td>
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<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$\rho (kg/m^3)$</td>
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<td>1.3</td>
<td>1.3</td>
<td></td>
</tr>
<tr>
<td>$c_s (m/s)$</td>
<td>328.17</td>
<td>328.17</td>
<td>328.17</td>
<td></td>
</tr>
<tr>
<td>$p_a (Pa)$</td>
<td>$1 \times 10^5$</td>
<td>$1 \times 10^5$</td>
<td>$1 \times 10^5$</td>
<td></td>
</tr>
<tr>
<td>$k (N/m)$</td>
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<td>2000</td>
<td>40500</td>
<td></td>
</tr>
<tr>
<td>$m (kg)$</td>
<td>0.8</td>
<td>0.8</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>$\omega_n (rad/s)$</td>
<td>100</td>
<td>50</td>
<td>225</td>
<td></td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td></td>
</tr>
<tr>
<td>$\omega (rad/s)$</td>
<td>341.6</td>
<td>334.8</td>
<td>376.0</td>
<td></td>
</tr>
<tr>
<td>initial piston velocity (m/s)</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>

Table 5-1 Parameters for FSI piston problems.

The FSI piston problem is first solved by the Euler equations and the fluid domain is divided into 100 cells (101 nodes). Fig. 5-2 shows the prediction of the piston displacement within 0.5 second using the velocity based coupling method at CFL=1. Fig. 5-3 and 5-4 shows the prediction of Blom’s (1998) research using stagger and monolithic schemes as comparison. One can clearly see that the velocity based method introduces less numerical damping compared to the other two methods. At higher CFL number (CFL=2, 5 and 10), the results are also plotted as comparison (Fig. 5-5, 5-6 and 5-7). The coupling piston frequencies of different cases are also listed in Table 5-2 for different CFL numbers. As the CFL number increases the damping of the piston displacement is also increasing. The frequency can be
predicted accurately at $\text{CFL} \leq 1$. The deviation of the frequency is not large when the CFL number increases. Blom (1998) claimed that the numerical damping of the results is mainly caused by the fluid solver and the transfer of the pressure between the fluid and solid. This study shows that the velocity based coupling algorithm tends to reduce the numerical damping caused by the interface pressure coupling efficiently.

Fig. 5-2 Displacement of piston at CFL=1, velocity based Euler.

Fig. 5-3 Displacement of piston at CFL=1, stagger (Blom, 1998).
Fig. 5-4 Displacement of piston at CFL=1, monolithical (Blom, 1998).

Fig. 5-5 Displacement of piston at CFL=2, velocity based Euler.

Fig. 5-6 Displacement of piston at CFL=5, velocity based Euler.
It can be observed from Fig. 5-7 that the equilibrium position of the piston deviates from 0 when the CFL number is high (CFL=10). This deviation was also captured by many previous researches (Blom, 1998; Michler et al, 2002; Michler et al, 2004). Many authors claimed that this non-physical deviation is caused by the less accurate prediction. The author considers this deviation is caused by the inaccurate initial boundary conditions for the values of pressure, velocity, density and energy. In order to produce more accurate predictions, small CFL values are preferred especially for unsteady cases. Fig. 5-8 show a damping history (10 seconds) of the piston displacement at CFL=1 with 51 nodes. This results show that when CFL is small, the non-physical deviation of the equilibrium piston position disappears.

In order to test the feasibility of the velocity based algorithm, two more cases are tested. Fig. 5-9 and 5-10 show the prediction of case b and c. For case b, which the coupling is much stronger since the spring frequency is only 50 rad/s, the result is still in a good agreement with the analytical solution. For case c, which the spring frequency itself is also high
(225 rad/s), the prediction can still distinguish the spring frequency and the coupling frequency.

![1D FSI Piston](image)

**Fig. 5-8** Displacement of piston at CFL=1, velocity based Euler.

<table>
<thead>
<tr>
<th>prediction of frequency for case a (rad/s)</th>
<th>CFL=1</th>
<th>CFL=2</th>
<th>CFL=5</th>
<th>CFL=10</th>
</tr>
</thead>
<tbody>
<tr>
<td>prediction of frequency for case b (rad/s)</td>
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<td>341.4</td>
<td>341.2</td>
<td>341.1</td>
</tr>
<tr>
<td>prediction of frequency for case c (rad/s)</td>
<td>334.7</td>
<td>334.6</td>
<td>334.5</td>
<td>334.2</td>
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<tr>
<td>prediction of frequency for case c (rad/s)</td>
<td>376.0</td>
<td>375.9</td>
<td>375.9</td>
<td>375.8</td>
</tr>
</tbody>
</table>

**Table 5-2** Comparison of predicted piston frequency.

Blom’s (1998) prediction showed that the result calculated by the acoustic equation 5-7, 5-8 and 5-9 has less damping than those by the Euler equation. The acoustic equations 5-7, 5-8 and 5-9 are also tested with the velocity based method to understand the feasibility of this method. Fig. 5-11 and 5-12 show the displacement calculated by discretization from equation 5-8 and 5-9 for case a. Both acoustic equations can predict the correct piston frequency at 341.6 rad/s. The two equations model tends to predict higher numeric damping.
than the Euler equations. This phenomenon is easy to understand, since the velocity based method is generated base on the Euler type equations. The two equations model (Equations 5-7 and 5-8) do not need to consider the velocity equation which make the solver as a stagger solver. The one equation model (Acoustic, Equation 5-9) tends to produce oscillation for the solution. The reason is the one equation model includes a second order time derivative of pressure. In addition, the one equation model condense all information in one equation; this may lead to unstable solution.

Fig.5-9 Prediction of case b at CFL=1, velocity based Euler.

Fig.5-10 Prediction of case b at CFL=1, velocity based Euler.
Fig. 5-11 Prediction of case a at CFL=1, velocity based Acoustic (Equation 5-7 and 5-8).

Fig. 5-12 Prediction of case a at CFL=1, velocity based Acoustic (Equation 5-9).

It should be pointed out that the current velocity based method is neither a monolithic type nor a stagger type scheme. The monolithic scheme considers solving a global matrix which linearized all the velocity components while the velocity based method considers a segregated solver for the x, y and z components of the velocity. Therefore, the current method is similar with the normal finite volume solver for fluid and can be further developed for 2D
and 3D FSI coupling.

5.3 Analysis of the key factors to the numeric coupling

Computational physicists always consider the accuracy of the model as a prime priority. Geometric conservation law (GCL) to the moving mesh of fluid (Thomas and Lombard, 1979; Demirdzic and Peric, 1990; Demirdzic and Peric, 1999) and interaction consistency law (ICL)(Blom, 1998) were developed to maintain the accuracy of the computational FSI problems. The authors would like to study the effect of these key factors into the coupling algorithm.

5.3.1 The effect of the GCL and mass accumulation to the moving mesh of fluid

The numeric simulations in the above sections are test by second order implicit temporal schemes, since the nature of the GCL indicates that the temporal discretization may cause mass accumulation in fluid. The authors also test the Lax explicit scheme and the first order implicit scheme for the same piston problem as comparison. The explicit scheme can only be stable at low CFL number (CFL ≤1), but the solution converge faster than the other methods. At high CFL number, the explicit scheme tends to predict a divergent piston displacement history which is cause by the numerical mass accumulation of the fluid part. On the other hand, the first order implicit scheme causes more numeric damping. Both these deviations are due to the mass imbalance of fluid caused by the dissatisfaction of the GCL for the moving mesh. In addition, first order approximation may lead to high numeric dissipation. Therefore,
higher order implicit temporal discretization which reduces the mass accumulation is a better selection for FSI prediction.

5.3.2 The effect of the ICL

For FSI prediction, the accuracy of the interface forces coupling is of crucial important. Blom (1998) introduced an interaction consistency law and indicated that the time dependence of the boundary conditions for FSI problem has to be consistent with the discrete time integration. The authors of this paper would like to develop the ICL further that the interface surface forces integration should also be consistent with the time integrated discretization.

First, the boundary velocity is consistent using equation 4-14. One can change this integration easily without the consistency as

\[ u^* = u_{\text{new}} \]  

(5-23)

The prediction shown in Fig.5-13 using this expression does not shows high numeric dissipation and dispersion compared to the original expression. It can be seen from equation 5-24 that the local piston pressure PL is also in a consistent form as

\[ p_L^* = \frac{1}{2} (p_{L\text{old}} + p_{L\text{new}}) \]  

(5-24)

If we test the inconsistent discretization like equation 5-23 as

\[ p_L^* = p_{L\text{new}} \]  

(5-25)

Fig.5-14 shows that the prediction using this inconsistent interface integration has quite large numeric damping. It can be concluded that the consistency of the surface force
integration at the interface is also important. Therefore, the FSI schemes should satisfy the
ICL for both boundary conditions and interface force coupling to predict accurate results. It is
clear that the velocity based FSI coupling algorithm satisfies the ICL at the boundary and the
interface.

Fig. 5-13 Displacement of piston at CFL=1, velocity non-consistent.

Fig. 5-14 Displacement of piston at CFL=1, pressure non-consistent.
5.4 Conclusion

A velocity based fluid-structure interaction algorithm has been presented. This algorithm is analyzed for a simple one dimension piston problem. The one dimensional non-linear Euler equations are chosen to model the compressible fluid. Arbitrary Lagrange Euler (ALE) method is used to handle the moving mesh of the fluid. The structure is integrated in time by the velocity based algorithm. The method shows good potential to solve the solid part. Since finite volume method is well documented in solving fluid, both fluid and solid are coupling implicitly within a single velocity based equation system and solved simultaneously.

The validation of the piston problem also shows the same advantage using the velocity based algorithm. This method tends to produce less numeric damping compared with the staggered scheme and the monolithical scheme. In addition, this method also performs well at high CFL number up to 10. The importance of the Geometric conservation law (GCL) for the moving mesh of fluid and the interaction consistent law (ICL) are also analyzed. The present analysis shows that the ICL that both boundary conditions and the interface integrations have to be consistent with the time dependence of the FSI solvers to avoid numerical damping.

The study shows the concept and the feasibility of a velocity based time marching fluid-structure interaction algorithm with moving mesh and nonlinear fluid equations. This method is tested in one dimensional manner. Since the formulation of the method is based on the Navier-Stokes equations. Therefore, this method can be easily obtained from existing fluid solvers for two dimensional and three dimensional cases.
Chapter 6

Modeling of Boundary Condition, Viscosity Model, Geometry and Hemodynamic in an Abdominal Aortic Aneurysm with Bifurcation

6.1 Introduction

To obtain valuable result of blood flow in the artery, it is required to set the viscosity model, boundary conditions and geometry accurately. As part of an effort to capture these phenomena, a pulsatile non-Newtonian blood flow in an AAA with bifurcated iliac artery is studied within this chapter. The primary objectives of this work are to have an in-depth understanding of the effectiveness and limitations of current state-of-art pulsatile flow models and viscosity models.

Most previous numerical studies applied simple pulsatile flat or parabolic inlet boundary conditions and Newtonian viscosity model in simplified geometries. Here, these analysis, by taking advantage of the most recent non-Newtonian modeling approach in conjunction with Womersley pulsatile boundary condition, are extended and validated to make the simulation more reliable.
6.2 Formulation

6.2.1 Basic Equations

The basic assumption of hemodynamic is that the flow is laminar and unsteady. The continuity and momentum equations (Navier-Stokes equations), are given as follows:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{6-1}
\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu) = \nabla \cdot \sigma \tag{6-2}
\]

where \( \rho \) is the density, \( u \) is the velocity vector, \( p \) is the pressure and \( \sigma \) is the stress tensor.

The stress tensor is related to the deformation tensor \( D \) and is represented as:

\[
\sigma = 2\eta(\dot{\gamma})D \tag{6-3}
\]

and

\[
D = \frac{1}{2}\left( \nabla u + \nabla u^T \right) \tag{6-4}
\]

where \( \eta \) represents the local viscosity of the blood and \( \dot{\gamma} \) is the shear rate.

6.2.2 Viscous Models

For Newtonian fluids such as water, the viscosity is always assumed to be constant. However, in complex fluids such as blood, which consists of plasma and particles, the viscosity can not always be considered constant. Plasma, which is made up of water (90%), dissolved proteins, glucose, mineral ions, hormones and carbon dioxide, can be assumed as a Newtonian fluid. The red blood cells (RBC) occupy 99% of the particulate volume of blood, and the remains 1% is made up of white blood cell, leukocytes and platelets. The red blood cells significant affect the blood rheology and make blood present shear thinning behaviour. Thus, the apparent viscosity of blood decreases as the shear rate increases. At low shear rate,
the aggregation of the RBCs make blood having a yield stress and high viscosity, while the realignment of blood cells at high shear rate causes low viscosity. In large healthy vessels with simple geometry and relatively high shear rate, blood can be assumed as a Newtonian fluid with a constant viscosity of $0.00345 \, Pa \cdot s$ (Cho and Kensey, 1991). In the abdominal aortic aneurysm with iliac bifurcation, the geometry is very complex, which causes high shear rate gradient near the aortic wall. Therefore, non-Newtonian models are needed to realistically predict the blood viscosity.

For a non-Newtonian fluid, $\eta$ is defined as a function of $\dot{\gamma}$. Yilmaz and Gundogdu (2008) presented a review on the various viscosity models used for blood flow in large arteries. The authors showed that time independent viscosity models are easy to use and achieve a reasonably good performance in calculating the wall shear stress. Carreau model of Johnston et al’s (2004) version is employed in this study. The effective viscosity is expressed as follow:

$$\eta = \eta_\infty + (\eta_0 - \eta_\infty) \left[ 1 + (\dot{\gamma}/\lambda)^2 \right]^{(n-1)/2}$$

(6-5)

where $\lambda = 3.313s$, $n=0.3568$, $\eta_0 = 0.056Pa \cdot s$ (viscosity at zero shear rate), $\eta_\infty = 0.00345Pa \cdot s$ (viscosity at infinite shear rate) (Cho and Kensey, 1991). In order to contrast the behaviour between Newtonian and non-Newtonian flows, numerical results using both the Newtonian and Carreau models will be presented later in this chapter.

### 6.2.3 Pulsatile Flow Physics

Pulsatile behaviour is a typical feature of the cardiovascular system. The pulsatile blood pressure nature significantly affects the aortic wall and the flow field. The majority of
numerical studies of AAA use empirical pulsatile velocity profile as the inlet boundary of AAA. Inlet velocity distribution at each time step is normally assumed to be parabolic by many researchers (Khanaf er et al., 2006; Li and Kleinstreuer, 2007). Moore et al. (1994) performed a comparison of in vitro and in vivo velocity measurement in a typical aortic channel. Their results showed that the velocity distributions do not necessarily display a parabolic behaviour. The authors also pointed out that the pulsatile effect can be expressed via the introduction of the Womersley number. Loudon and Tordesillas (1997) tried to use the Womersley number to characterize the pulsatile internal flow employing the oscillating pressure gradient. Their analysis showed that when the Womersley number is high (i.e., Wo=10), the velocity distribution can not be assumed to be parabolic. The Womersley number in the large artery like the abdominal artery is around 10. Thus, assuming a parabolic profile at the inlet during the whole cardiac cycle is not a realistic hypothesis. In this study, a more realistic inlet velocity distribution based on the Womersley theory (Womersley, 1955) is developed and applied to simulate the pulsatile blood flow.

In this study, a waveform of the volume flow rate (Fig. 3-1a) as reported by Olufsen et al. (2000) is used at the inlet. The authors also presented an outlet pressure profile (Fig. 3-1b) corresponding to the iliac arteries. The heart beat rate in this study is assumed to be 70 beats per minute (0.857s per cycle, T=0.857s), and the blood density is assumed to be 1060 kg/m$^3$. According to the inlet volume flow rate, a simple relation assuming constant radius can be employed to obtain the mean blood velocity at the inlet section as:

$$v_{\text{mean}}(t) = \frac{q(t)}{\pi (d/2)^2}$$

where d is the aortic diameter, t is time. Some authors recently (Khanaf er et al., 2006; Li and
Kleinstreuer, 2007) assumed a parabolic velocity distribution at the inlet in the following form:

\[ v(r, t) = 2v_{\text{mean}}(t) \left[ 1 - \left( \frac{2r}{d} \right)^2 \right] \]  

(6-7)

where \( r \) is the radius position of the aortic channel, \( v_{\text{mean}} \) is the mean velocity. However, the above form can not realistically represent pulsatile behaviour. In the classic research carried out by Womersley (1955), a theory is developed to approximate the laminar pulsatile flow profile. Blood flow rate is relatively easy to measure experimentally. Thus, an expression of pulsatile velocity can be deduced according to the Womersley theory. A periodic function of volume flow rate can be defined from the data of Fig. 6-1(a), as given by the following expression:

\[ Q(t) = A_0 + \sum_{m=1}^{m=12} A_m \cos mw t + \sum_{m=1}^{m=12} B_m \sin mw t \]  

(6-8)

where \( w \) is defined as

\[ w = \frac{2\pi B_{\text{heart}}}{60} \]  

(6-9)

and \( B_{\text{heart}} \) is the heart beats per minute. If the full period is taken as \( 2\pi \), the measured values of volume flow rate \( q_r \), \( r=0,1,2,...,23 \) at 24 equally sampled points (\( \pi/12 \) apart) are required to calculate the coefficients. Thus,

\[ A_0 = \frac{1}{24} \sum_{r=0}^{r=23} q_r , \]  

(6-10)

\[ A_m = \frac{1}{12} \sum_{r=0}^{r=23} q_r \cos mr \cdot 15^\circ , \]  

(6-11)

\[ B_m = \frac{1}{12} \sum_{r=0}^{r=23} q_r \sin mr \cdot 15^\circ ; \]  

(6-12)

Writing the flow rate using a Fourier analysis, one can obtain
\[ Q(t) = A_0 + \sum_{m=1}^{m_{max}} \sqrt{A_m^2 + B_m^2} \sin(wmt + \delta_m) \]  
\[ \delta_m = \arctan \frac{A_m}{B_m} \]  

Similar methods can be used to work out the periodic nature of the outlet pressure waveform.  

Considering a pressure gradient at the inlet as the real part of a complex valued series:

\[ \frac{\partial p}{\partial x} = \text{real} \left[ \sum_m P_m e^{i\omega m u} \right] \]  
\[ \frac{\partial p}{\partial x} = \sum_m M_m \cos(mw t + \phi_m) \]  

Womersley (1955) provided a solution of the velocity function based on this pressure gradient function, as given by:

\[ u(r, t) = \text{real} \left[ \sum_m \frac{1}{\rho i \omega m} \left\{ 1 - \frac{J_0 \left( \frac{Wo \cdot r / R \cdot i^{3/2}}{R} \right)}{J_0 \left( \frac{Wo \cdot i^{3/2}}{R} \right)} \right\} e^{i\omega m u} \right] \]  

where \(Wo\) is the Womersley number defined as

\[ Wo = R \sqrt{\frac{W}{\nu}} \]  

\( \nu \) is the fluid kinetic viscosity, \( R \) is the radius of the artery, \( \rho \) is the fluid density, and \( J_0(\xi R^{3/2}) \) is a Bessel function of order zero. If we express the Bessel function in the form of a corresponding modulus and phase as:

\[ J_0 \left( \frac{Wo \cdot r / R \cdot i^{3/2}}{R} \right) = M_0 \left( \frac{r}{R} \right) e^{i\theta_0(r/R)} \]  
\[ J_0 \left( \frac{Wo \cdot i^{3/2}}{R} \right) = M_0 e^{i\theta_0} \]

Then the corresponding velocity can be expressed as
\[ u(r, t) = \sum_m \left[ \frac{P_m}{\rho \, \omega m} \left( \sin(wmt + \phi_m) - \frac{M_0(r/R)}{M_0} \sin(wmt + \phi_m - \delta_0) \right) \right] \]  

(6-21)

where

\[ \delta_0 = \theta_0 - \theta_0(r/R) \]  

(6-22)

Rearranging the above equations one obtains:

\[ u(r, t) = \sum_m \left[ \frac{P_m}{\mu \, \omega^2} \frac{R^2}{M_0} \sin(wmt + \phi_m + \varepsilon_0) \right] \]  

(6-23)

\[ h_0 = \frac{M_0(r/R)}{M_0} \]  

(6-24)

\[ M_0' = \sqrt{1 + h_0^2 - 2h_0 \cos \delta_0} \]  

(6-25)

\[ \tan \varepsilon_0 = \frac{h_0 \sin \delta_0}{1 - h_0 \cos \delta_0} \]  

(6-26)

The volume flow rate can be provided by integrating the velocity in the form of:

\[ Q = 2\pi \int_0^\kappa u(r, t) rdr \]  

(6-27)

This can be simplified employing the particular properties of Bessel functions to yield:

\[ Q = \sum_m \left[ \frac{\pi R^4}{\mu \, \omega^2} \frac{P_m}{W_0^2} \left( \sin(wmt + \phi_m) - \frac{2M_1}{W_0M_0} \sin(wmt + \phi_m - \delta_{10}) \right) \right] \]  

(6-28)

\[ J_1(W_0 \cdot i^{3/2}) = M_1 e^{i\theta} \]  

(6-29)

\[ \delta_{10} = 135^\circ - \theta_1 + \theta_0 \]  

(6-30)

This may be reduced to a single-phase relationship by defining:

\[ Q(t) = \sum_m \left[ \frac{\pi R^4}{\mu \, \omega^2} \frac{M_{10}}{W_0^2} P_m \sin(wmt + \phi_m + \varepsilon_{10}) \right] \]  

(6-31)

\[ k = \frac{W_0M_0}{2M_1} \]  

(6-32)

\[ M_{10}' = \frac{1}{k} \sqrt{\sin^2 \delta_{10} + (k - \cos \delta_{10})^2} \]  

(6-33)
\[
\tan \epsilon_{10} = \frac{\sin \delta_{10}}{k - \cos \delta_{10}} \quad (6-34)
\]

The modulus and phase of the pressure gradient can be obtained by comparing the empirical flow rate expression to the single-phase Womersley flow rate solution. Thus:

\[
P_m = \frac{\mu \omega_0^2 \sqrt{A_m^2 + B_m^2}}{\pi R^4 M_{10}} \quad (6-35)
\]

\[
\phi_m = \delta_m - \epsilon_{10} \quad (6-36)
\]

Hence the pulsatile velocity distribution can be expressed in the following explicit form relationship:

\[
u(r, t) = u_0(r) + \sum_{m=1}^{m=12} \left[ \frac{P_m}{\mu \omega_0^2} \frac{R^2}{M_0} \sin(wmt + \phi_m + \epsilon_0) \right] \quad (6-37)
\]

where

\[
u_0(r) = \frac{2A_0}{\pi R^2} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (6-38)
\]

The originality of this method is reproducing the pressure gradient expression (Equation 6-16 and 6-35) using empirical volume flow rate. The 2D and 3D Womersley velocity distribution can then be calculated with the computed pressure gradient. An in-house Fortran code was developed to produce this pulsatile velocity distribution using the patient-specific volume flow rate, and a C++ User Defined Function (UDF) was coded to input this velocity profile into Fluent. Since the pressure fields at both iliac bifurcations do not display significant differences, identical pressure waveforms are applied at the two outlets for the three-dimension analysis. However, it is well known that small changes in pressure field will directly affect the flow field. In order to test for the imbalance pressure influences at the outlets on the evolving internal flow field, pressure waveforms with 0.05% differences are
used at the two bifurcations. In addition, the artery walls are assumed to be rigid with no velocity slip in this study.

(a) inlet  
(b) outlet  
Fig. 6-1 Inlet flow rate and the outlet pressure waveform (Olufsen et al., 2000).

6.2.4 AAA Geometrical Models

2D AAA geometrical models are employed to provide numerical simulation configurations. The aneurysm is naturally described by the following parameters: the aneurysm length $L$, the AAA neck length $l_{\text{neck}}$, the un-dilated aortic diameter $d$ and the maximum diameter $D$. The geometry of the aneurysm can be approximated by the following function:

$$y = \frac{d}{2} + \frac{D - d}{4} \left[ 1 - \cos \left( \frac{2\pi x}{L} \right) \right], \quad 0 \leq x \leq L$$

(6-39)

In order to specify the aneurysm size, the dilation ratio $D/d$ and dimensionless length $L/d$ are introduced. Clinical results showed that the average un-dilated aortic diameter is around 20mm, and the length of the aneurysm is around 4 times the un-dilated aortic diameter. Since the rupture rate is relative high when the maximum diameter of the aneurysm is above 6mm,
the dilation ratio $D/d=3$ is selected. Fig. 6-2 shows a 2D axisymmetric AAA model with $D/d=3$, $L/d=4$, $l/d=1$ and $d=20$ mm. The mesh and boundary conditions are shown in Fig. 6-3.

![Fig. 6-2 2D axisymmetric AAA model.](image)

![Fig. 6-3 Mesh and boundary conditions of 2D axisymmetric AAA model.](image)

A 3D AAA bifurcating model is described by the following geometric parameters: length $L$, the AAA neck length $l$, the un-dilated aortic diameter $d$, the maximum diameter $D$, the iliac diameter $d_i$ and the iliac bifurcation angle $\phi$. In order to specify the AAA bifurcation geometry, the parameters used in the calculation are shown in Table. 6-1. Gordana et al. (2008) introduced a cases study report and claimed that the maximal aortic diameter and the aneurysm expansion rate are the best predictor factor for rupture of the AAA. An estimated five-year rupture rate is up to 35% when the diameter of the AAA is 6.0 to 6.9 cm. In this study, a simply symmetric AAA model with a maximal aortic diameter of 6.0 cm and a bifurcation angle of $60^\circ$ is tested. Fig. 6-4 and 6-5 shows the 3D geometry and mesh of the
bifurcation AAA model.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>d (mm)</th>
<th>di (mm)</th>
<th>D/d</th>
<th>L/d</th>
<th>l/d</th>
<th>φ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values</td>
<td>20</td>
<td>14</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>60°</td>
</tr>
</tbody>
</table>

Tab.6-1 Geometry parameters used in the calculation.

Fig. 6-4 Geometry and mesh of the 3D AAA bifurcation model.

Fig. 6-5 Mesh of the 3D AAA bifurcation model.
6.2.5 Numerical Schemes and Initial Conditions

Fluent (Ansys, Inc, 2012) is a commercial CFD tool able to handle such complex three dimensional flows. The governing equations are solved employing a second order UPWIND scheme, while the SIMPLE and PISO algorithms were employed to couple the pressure and velocity fields (SIMPLE for steady cases, PISO for unsteady cases). In order to implement the various inlet and outlet boundary conditions, a simple User Defined Function (UDF) was coded to read the coefficients output from the Fortran code. Steady flow fields with inlet and outlet boundary conditions at a given time by Eqn. 6-37 are taken as the initial guess. At each time step, when the residuals of continuity and momentum equations reach levels less than $10^{-6}$, the convergence criteria were deemed satisfied. Two more cardiac cycles are calculated once the resulting fields display stationarity as verified by the monitoring typical values i.e., velocities possessing identical phases in two neighbouring periods reach the same level (differences less than 1%).

Before converging on validated final simulations, the mesh-independence of the predictions (3D) was checked using different meshes (medium, coarse, fine and very fine meshes of 222412, 112342, 312474 and 434428 control volumes (CVs) respectively). Fig. 6-6 shows the grid-independence comparison of centre line velocity distribution of the AAA in different meshes. The results do not improve so much when the meshes increase. The medium mesh (222412 CVs) works very well for the simulation. In order to improve the compute efficiency, all the results shown in this study are based on the mesh of 222412 CVs.
6.2.6 2D Aneurysm Flow Analysis and Validation

Numerical results were validated to show the viability of the numerical methods employed in this study. The 2D AAA model was set to be axisymmetric. Budwig et al. (1993) presented an experimental study of blood flow in a 3D axisymmetric rigid AAA model. A comparison of the velocity profiles across the centre line of the aneurysm between numerical results (present and Khanafer et al., 2006) and the experimental data of Budwig et al. (1993) for a steady blood flow with Reynolds number of 400 is illustrated in Fig. 6-7. The blood viscosity is assumed to be constant as \(0.00345 \text{Pa} \cdot \text{s}\). The present calculations show a good agreement with two previous studies. Fig. 6-8 also shows that the calculated wall shear stresses match the previous experimental measurements. These comparisons do support the conclusion that the numerical results produce by Fluent in this study display a reasonable level of agreement when compared with experimental measurements. In addition, the present
numerical method in Fluent can successfully predict the wall shear stresses field along the aneurysm surface.

Fig. 6-7 Comparison of velocity distributions across the centre line for AAA (solid: present numerical results; dash: numerical results of Khanafer et al. (2006); square: experimental results of Budwig et al. (1993)).

Fig. 6-8 Comparison of the predicted wall shear stresses vs experimental measurements of Budwig et al. (1993).
One of the purposes of this study is to use the dimensionless Womersley number to characterize the pulsatile flow inlet conditions. In order to capture the pulsatile development of the flow just downstream of the inlet, velocity distributions close to the inlet (x=20mm) are presented for both Womersley and parabolic inlet conditions. Fig. 6-9 shows a comparison of the radial velocity profiles at x=0mm and x=20mm between two inlet conditions. The pulsatile blood flow is spatially well developed before the aneurysm. Thus, the shapes of the velocity profiles at two nearby locations prior to the aneurysm do not display substantial differences. As shown in Fig. 6-9, the shape of the Womersley inlet velocity profile matches the velocity profile captured at x=20mm during the whole heart beat period. Quantitative discrepancies of magnitude between the two positions are due to the pulsatile flow rate effect. However, the parabolic inlet velocity profile is significantly different from the Womersley velocity profile at x=20mm except when the flow is accelerating. Further, the velocity profile at x=20mm using the parabolic inlet condition matches the shape of the Womersley inlet profile. These results indicate that the parabolic inlet velocity profile still needs to be developed a-priori through the calculation. This also means that the parabolic boundary condition needs extra calculation domain of the AAA neck to obtain a fully developed velocity field goes into the AAA while the Womersley boundary can do this with a shorter AAA neck. Therefore, the Womersley velocity distribution can provide a better approximation at the inlet and it can reduce computational resource. Fig. 6-9 also shows the comparison for velocity fields at peak systole (t/T=0.23) between the two inlet conditions.
Fig. 6-9 Comparison of the velocity profiles at x=0mm and x=20mm between the Womeraley and the parabolic inlet conditions.
The comparison of velocity vectors and contours plots between the Womersley and parabolic inlet condition at peak systole (t/T=0.23) is illustrated in Fig. 6-10. Since the flow is still not well developed before the aneurysm using the parabolic condition, the velocity prediction at the axis is higher than the results using the Womersley theory. This may lead to an unreasonable estimation of the whole flow field. One can lengthen the aneurysm neck calculation domain to obtain the Womersley distribution at before the aneurysm using parabolic inlet, but this will waste additional computational resource.

Fig. 6-10 Comparison of velocity vectors and contour plots between the Womersley and the parabolic inlet.

The influence of inlet condition on the wall shear stress is also a primary concern of practical stent manufacturers. Fig. 6-11 (a, b, c) illustrate the shear stress comparisons between the two inlet conditions at three times (t/T=0.17s, t/T=0.23s, t/T=0.28s).
Fig. 6-11 Comparison of the wall shear stress between the two inlet conditions at three time phases (a: $t/T=0.17$; b: $t/T=0.23$; c: $t/T=0.28$).
At the middle of the aneurysm \((-3.0 \leq x/d \leq 3.0\), shear stress predictions with both inlets are similar. However, the shear stresses near the proximal end \((x/d \leq -4.0\) ) differ significantly between two conditions. These are related to the previously displayed fields that the flow is not well developed with the parabolic inlet. The neck length of the AAA varies significantly for different patients with some having a very short AAA neck. Using the parabolic inlet for these cases is not a good approximation as the neck length before the aneurysm is not long enough to let the flow develop fully. Hence, the Womersley inlet condition can provide an inlet assumption in line with pulsatile blood flow behaviour with a shorter AAA neck computation domain.

In this study, using the parabolic inlet condition gave rise to comparatively more difficult convergence behaviour to reach the periodic stationary conditions, i.e., takes more time steps per run to reach the periodic stationary condition using the parabolic inlet as compared with the Womersley inlet. The reason for this is using parabolic inlet boundary which is not a fully developed assumption of pulsatile flow needs additional calculation time to reach the stationary condition. The Womersley inlet conditions provided in this study are also easy to employ with an insignificant pre-calculation step cost (applying the user defined function) before each overall time step.

This section mainly focuses on numerical predictions obtained with the Womersley inlet condition that presents a more reasonable pulsatile flow field. The viscosity of blood is assumed constant in the previous calculation. Non-Newtonian effect is also very important to produce good results, thus non-Newtonian models are applied as compared with the Newtonian model. Fig. 6-12, 13, 14 and 15 show the blood flow fields (vectors and contour)
predicted using Newtonian and non-Newtonian models employing the same Womersley inlet conditions. A recirculation vortex near the distal end of the aneurysm can be observed at $t=0.0s$ in both models. For the Newtonian model, a weaker secondary vortex occurs close the centre of the aneurysm, while the non-Newtonian model displays no such secondary vortex. This is due to the non-Newtonian effect on properties such as the local viscosity that displays much higher numerical values. Changes of the velocity at the early systolic period ($0<t/T<0.12$) are not significant, thus, the flow fields between $t/T=0$ and $t/T=0.12$ do not show great differences. After $t/T=0.12$, the flow starts to accelerate. The recirculation vortex becomes weaker at $t/T=0.17$ and disappears near the peak systole ($t/T=0.23$). The entire flow field then develops to exit channel without any substantial reversal at this time. The velocity gradients near the aortic wall at both the proximal and distal ends also reach peaks at $t/T=0.23$. The flow then decelerates in the period between $0.23<t/T<0.53$, a new recirculation vortex appears and starts developing in this period. At the diastolic phase ($0.53<t/T<1.0$), the new vortex moves from the proximal to the distal end of the aneurysm. In the period between $0.53<t/T<0.65$ when the flow rate direction is negative (towards the inlet), the flow near the axis of the aneurysm is still outgoing. This distribution matches the inlet Womersley condition. Previous numerical study of Khanafer et al. (2006) using the parabolic pulsatile inlet condition also presented similar Womersley like phenomena. Therefore, using the Womersley theory can provide a better approximation of the inlet velocity distribution. The flow accelerates again after $t/T=0.65$ and the new vortex becomes weaker and weaker in this period. The flow develops to evolve to another cycle by the end of this cycle ($t/T=1.0$), the above phenomenon thus repeats periodically during each successive cycle.
Fig. 6-12 Velocity vector plots for AAA at different time periods (t/T=0,0.12,0.17,0.23,0.28).
Fig. 6-13 Velocity vector plots for AAA at different time periods ($t/T=0.41,0.53,0.65,0.76,0.88$).
Fig. 6-14 Velocity contour plots for AAA at different time periods (t/T=0,0.12,0.17,0.23,0.28).
Fig. 6-15 Velocity contour plots for AAA at different time periods (t/T=0.41,0.53,0.65,0.76,0.88).
The non-Newtonian effect is significant during the whole heart beat cycle. The radial velocity distribution near the axis for the non-Newtonian model is substantially more flat compared with the Newtonian model. The higher viscosity due to the zero velocity gradients at the axis cause higher resistance to the shear flow development. The higher resistance is caused by the red blood cell accumulation in the middle of the artery when the velocity of blood is high (large Womersley number). In addition, higher viscosity tends to display less energetic flow activity as most structures are damped. Hence, the Newtonian model (lower viscosity) exhibits two vortices, while the non-Newtonian displays only one. Fig. 6-16 also demonstrates the wall strain rate distribution comparison between the Newtonian and the non-Newtonian model. The strain rate differs significantly at the main aneurysm ($-3.5 \leq x/d \leq 3.5$). This means that the non-Newtonian model influences the flow field within the aneurysm body where the geometry is complex.

Fig. 6-17 illustrates the distribution of shear stress along the aortic wall at peak systole ($t/T=0.23$). The predictions show that shear stress peak at both the proximal and distal ends reach low levels near the centre of the aneurysm. Shear stress distributions before and after the peak systole are also shown in Fig. 6-18 and 6-19. Comparisons show that the wall shear stress reaches a maximum at peak flow. Furthermore, the non-Newtonian model tends to provide higher numerical values of shear stress compared with the Newtonian model. This can be appreciated as being due to the fact that the local viscosity of the non-Newtonian model is higher as compared with the Newtonian model. The WSS difference is not just a constant increase. The WSS difference is not large in the middle of the aneurysm while this difference becomes clearer near the proximal and distal end. Hence, one cannot just artificial
increase the Newtonian viscosity in the calculation to obtain the correct WSS as the change is not linear. However, the global shear stress is not always higher for the non-Newtonian model, as the local shear rate also influences the shear stress values (Fig. 6-16). Another simple power law model was also employed to provide predictions. The power law model gives similar results as the Newtonian model near the centre of the aneurysm, where the shear rate is low. Thus, a simple power law model is not suitable to present the non-Newtonian rheology of blood. It is also easily appreciated that the wall shear stress changes significantly at both the proximal and the distal ends. The oscillatory nature of wall the shear stresses accompanied with the pulsatile pressure nature contributes significantly to the growth of AAA over a long period.

Fig. 6-16 Radial strain rate distribution for different viscosity models after peak systole ($t/T=0.28s$).
Fig. 6-17 Wall shear stress distribution for different viscosity models at peak systole (t/T=0.23s).

Fig. 6-18 Wall shear stress distribution for different viscosity models at t/T=0.17s.
In conclusion, the effect of the parabolic and Womersley inlet conditions on the pulsatile flow field within AAA model has been numerically studied. The predictions demonstrate that the Womersley condition is a better assumption for use as the inlet condition for pulsatile blood flow compared with the parabolic inlet. With the parabolic inlet which is not always well developed, the wall shear stress at the proximal end may not be predicted accurately, in some cases displaying a completely wrong behaviour.

The analysis of blood flow with different viscosity models demonstrates that the non-Newtonian nature of blood rheology has significant influences on the flow field evolution. The non-Newtonian properties tend to lead the flow to a reach more flat field behaviour under the assumed pulsatile conditions. The effect concerning the aortic wall shear stress for the non-Newtonian rheology can not be neglected in estimating the rupture risk of
AAAs. Wall shear stress was found to reach a peak at both the proximal and the distal ends of the aneurysm. Moreover, the shear stresses within these regions display rapidly changing profiles during the whole cardiac cycle. This may contribute substantially to the growth of the AAA as well as the oscillating pressure field.

6.2.7 Results of 3D Aneurysm with Bifurcation

The reliability of the Womersley inlet velocity distribution is of utmost importance in this study. As discussed in the previous session, the Womersley inlet captures reliably the well developed pulsatile behaviour. Numerical results for the 3D Aneurysm model with bifurcation is presented in this section. Mid-plane blood flow patterns at distinct time levels ($t/T=0.0$, $t/T=0.17$, $t/T=0.23$ and $t/T=0.28$) during the cardiac cycle are shown in Fig. 6-20 and 6-21. The flow of blood at the inlet starts accelerating from $t/T=0.0$ and peaks at $t/T=0.23$. During this period no vertical structure appears at the proximal end of the aneurysm, these results also match the 2D analysis. The $y$ and $z$ direction radial velocity profiles in the centre of the aneurysm are shown in Fig. 6-22. In order to understand the hemodynamic at the end of systole, Fig. 6-23 and 6-24 presents the mid-plane velocity vector and contour plots during the period from $t/T=0.28$ to $t/T=0.52$. Vortices are observed and start developing while the blood flow is decelerating.
Fig. 6-20 Mid-plane blood flow patterns in the neck of the aneurysm at different time levels ($t/T=0.0$, $t/T=0.17$, $t/T=0.23$ and $t/T=0.28$).

Fig. 6-21 Velocity vector plots at peak systole ($t/T=0.23$).
Fig. 6-22 Radial velocity distribution along y and z axis in the middle of the aneurysm at $t/T=0.17$ and $t/T=0.23$.

Fig. 6-25 and 6-26 illustrate the non-Newtonian effects on the evolution of the flow fields and wall shear stress distribution. The results show that the non-Newtonian model tends to predict a much smaller vortex. Fig. 6-27 present the skin friction coefficient prediction differences between Newtonian and non-Newtonian models. The non-Newtonian model tends to predict higher WSS especially in the bifurcation point compared with the Newtonian model. Strain rate distributions in the middle of the AAA are also investigated in Fig. 6-28, 6-29 and 6-30. It can be observed that a more uniform strain rate distribution can be obtained using the non-Newtonian model. The strain rate differences near the artery wall are very large between the two models. This result matches the finding obtained from the 2D simulation. Normally the red blood cells accumulate in the middle of the artery, which make the strain rate more uniform near the centre line. Therefore, the non-Newtonian model has a better performance to predict the rheology of the blood.
Fig. 6-23 Mid-plane velocity vector plots at $t/T=0.28$, $t/T=0.41$ and $t/T=0.52$. 
Fig. 6-24 Mid-plane velocity contour plots at $t/T=0.28$, $t/T=0.41$ and $t/T=0.52$. 
Fig. 6-25 Comparison of velocity vector predictions between Newtonian and non-Newtonian models.
Fig. 6-26 Comparison of velocity contour predictions between Newtonian and non-Newtonian models.
Fig. 6-27 Comparison of skin friction coefficient distributions between Newtonian and non-Newtonian models at t/T=0.23.

Fig. 6-28 Comparison of strain rate distributions in the middle of the AAA between Newtonian and non-Newtonian models at t/T=0.23.
Fig. 6-29 Comparison of strain rate distributions in the middle of the AAA (centre line at y direction) between Newtonian and non-Newtonian models at $t/T=0.23$.

Fig. 6-30 Comparison of strain rate distributions in the middle of the AAA (centre line at z direction) between Newtonian and non-Newtonian models at $t/T=0.23$. 
Fig. 6-31 and 6-32 show the strain rate and skin friction coefficient distribution at different time phases of the cardiac cycle. It is easily observed that wall shear stress varies significantly near the proximal end, the distal end and the bifurcation point. These findings match the 2D results in the previous section. At the peak systole, the artery wall experiences the greatest shear stress. Somewhat remarkable is the fact that the wall shear stress peaks at the two iliac bifurcations right after the bifurcation point, while zero shear stress is observed at the bifurcation point.

![Strain Rate 1/S](image)

Fig. 6-31 Wall strain rate distributions at t=0.20s and t=0.65s.
Fig. 6-32 Skin friction coefficient distribution during the cardiac cycle (non-Newtonian model).
The outlet pressure at both iliac arteries are set to be equal in the first test, while the real blood pressure conditions are not balance. Fig. 6-33 and 6-34 illustrates the flow patterns with an unbalanced pressure outlet, where the outlet pressure on one of the iliac segments (the bottom one) is 0.05% higher than the other one. It is easily observed that the overall flow field before the bifurcation does not display significant differences as compared to the balanced pressure case. During acceleration ($t/T=0.17$ and $t/T=0.23$), the flow patterns between the two iliac bifurcations are similar. The upper artery which has the lower outlet pressure comprises higher velocity magnitudes. When the flow decelerates, a much stronger reverse flow occurs in the bottom artery. The imbalance pressures also affect the flow in the middle of the aneurysm where a larger vortex occurs. The wall shear stress distribution of the iliac arteries is also illustrated in Fig. 6-35. The flow dynamics within the AAA (Non-Newtonian viscous properties and boundary conditions) affects the magnitude of the maximum wall shear stress rather than its location. Table. 6-2 shows an overall comparison of maximum WSS between different viscosity models and boundary conditions during a cardiac cycle. The comparison between non-Newtonian and Newtonian model yields a maximum 42% difference in WSS, while Newtonian model tends to have a 7.7% underestimation of WSS at peak systole. Numerical results also show that imbalance outlet pressure condition provides a higher peak WSS (maximum 26.2%).
Fig. 6-33 Comparison of velocity vector plots between equal and unequal outlet pressure conditions.
Fig. 6-34 Comparison of velocity contour plots between equal and unequal outlet pressure conditions.
Fig. 6-35 Wall shear stress distributions for unequal outlet pressure at different time phases.
<table>
<thead>
<tr>
<th></th>
<th>t=0.00s</th>
<th>t=0.10s</th>
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<th>t=0.25s</th>
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<tr>
<td>Peak WSS for Non-Newtonian model (Pa)</td>
<td>1.50</td>
<td>1.06</td>
<td>16.69</td>
<td>14.88</td>
<td>3.14</td>
</tr>
<tr>
<td>Peak WSS for Newtonian model (Pa)</td>
<td>1.53 (2.0%)</td>
<td>1.07 (9.5%)</td>
<td>16.11 (-3.5%)</td>
<td>13.74 (-7.7%)</td>
<td>3.18 (1.3%)</td>
</tr>
<tr>
<td>Peak WSS for imbalance outlet pressure (Pa)</td>
<td>1.61 (7.3%)</td>
<td>1.32 (24.5%)</td>
<td>18.03 (8.0%)</td>
<td>15.39 (3.4%)</td>
<td>3.15 (0.3%)</td>
</tr>
<tr>
<td>Peak WSS position</td>
<td>D</td>
<td>D</td>
<td>B</td>
<td>P &amp; B</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
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<th>t=0.55s</th>
<th>t=0.65s</th>
<th>t=0.75s</th>
<th>t=0.85s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak WSS for Non-Newtonian model (Pa)</td>
<td>1.71</td>
<td>0.61</td>
<td>1.00</td>
<td>1.59</td>
<td>1.53</td>
</tr>
<tr>
<td>Peak WSS for Newtonian model (Pa)</td>
<td>1.68 (-1.8%)</td>
<td>0.51 (-16.4%)</td>
<td>1.42 (42.0%)</td>
<td>1.96 (23.3%)</td>
<td>1.53 (0.0%)</td>
</tr>
<tr>
<td>Peak WSS for imbalance outlet pressure (Pa)</td>
<td>1.66 (-2.9%)</td>
<td>0.77 (26.2%)</td>
<td>1.24 (24.0%)</td>
<td>1.56 (-1.9%)</td>
<td>1.57 (2.6%)</td>
</tr>
<tr>
<td>Peak WSS position</td>
<td>P &amp; D</td>
<td>D &amp; B</td>
<td>D &amp; B</td>
<td>D</td>
<td>D</td>
</tr>
</tbody>
</table>

Tab. 6-2 Comparison of maximum wall shear stress (in Pa) within the AAA among the three conditions (Non-Newtonian model, Newtonian model and imbalance outlet pressure). The parentheses show the % difference of the stress obtained with the Newtonian and imbalance outlet pressure conditions with respect to the Non-Newtonian balance outlet pressure condition. (P: Proximal end; D: Distal end; B: around Bifurcation point)

### 6.2.8 Discussion of the 3D results

At the three distinct time phases (Fig. 6-20), the corresponding shapes of the axial velocity distribution at the inlet and before the aneurysm are similar. Thus Womersley solution tends to provide a better approximation for the fully developed pulsatile pipe flow compared with the parabolic assumption. These conclusions are in line with the results from the previous study for the 2D AAA model. At the peak systole (t/T=0.23), no reverse flow occurs in the aneurysm, while a vortex appears at the distal and proximal end of the aneurysm before and after the maximum inflow. In the middle of the aneurysm, blood proceeds predominantly in the axial direction, while it further separates into two streams at a location...
corresponding to the two iliac arteries inside the slice C-C’ (Fig. 6-21). This shows clearly that the bifurcation directly affects the flow field evolution upstream of the bifurcating region. Fig. 6-22 also shows that the y and z axial velocity profiles in the centre of the aneurysm are not identical. Thus, the geometry of the bifurcation region has a prime effect on the upstream flow details. It is also clear that the secondary flow effects near the bifurcating region are also much stronger than in the aneurysm. Therefore, the effect of the bifurcation region can not be neglected. This also indicates that numerical calculations for 2D or 3D AAA models without bifurcation region can not provide the full details of the flow field.

At the end of systole (t/T=0.52), maximum backflow occurs at the inlet. From t/T=0.23 to t/T=0.52 (Fig. 6-23 and 6-24), the flow starts decelerating, reverse flow appears at the outer side of the iliac outlet. The reverse flow subsequently becomes stronger and finally occupies the whole outlet. The velocity distribution at the outlet also shows that the reverse velocity field at the outer side is higher than the inner side, in line with the presumed shape of the pulsatile inlet profile.

In order to capture the effect of this aspect of non-Newtonian behaviour on the pulsatile flow details in the AAA, a comparative study between the Newtonian and non-Newtonian models is presented. The non-Newtonian model also presents a far more uniform axial velocity near the axis. The reason of this is that, near the axis the shear rate is comparatively low giving rise to high viscosity values due to the shear thinning behaviour. The comparison of wall shear stress distribution also demonstrates that the Newtonian model may under predict the peak wall shear stress at peak systole. The maximum difference of maximum WSS prediction between these two models is up to 42% at t/T=0.76. Thus, the
non-Newtonian effects can not be neglected in a rigorously formulated computational method.

The high wall shear stress is primarily caused by the local high strain rate (Fig. 6-31). The rapidly changing behaviour of the wall shear stress at both the proximal and distal ends with accompanying oscillating pressure fields contribute to the growth of the aneurysm. Indeed, as reported by Golledge et al. (1999) 73% of the AAA rupture cases occur in the middle third near the distal end. During the whole cardiac period, WSS peak at the distal end of the AAA except at the peak systole. Aneurysm in the iliac aortic is also found post bifurcation in many patients. The maximum wall shear stress near the bifurcation point may potentially explain the reason for this.

The role of WSS to the rupture risk of the AAA is often ignored because its magnitude is far less than the normal-acting wall stress. However, AAA development is a long term effect. Therefore, the patterns of WSS in Fig. 6-27 and 6-32 represent the WSS which likely can be correlated to the growth of the aneurysm. WSS also plays an important role to stent graft migration. Litwinski et al. (2005) reported that stent graft migration and aortic neck elongation may cause loss of proximal fixation. According to the results from Tab. 6-2, WSS also changes rapidly at the proximal end of the aneurysm which may contribute to the elongation of the aortic neck.

Normally, the outlet pressure values in the two iliac bifurcations are assumed to be equal. In vivo experiments also show that the pressure difference between two outlets is small. However, the pressure significantly influences the flow field, with a small difference producing remarkable changes within the flow field. Pressure differences between two iliac
bifurcations may be due to a variety of reasons (i.e. different iliac artery diameter; blood blockage, etc). Patients with iliac aneurysm may have different pressure in two iliac arteries. Thus the effect of imbalance outlet pressure is being studied in this study.

Since the upper iliac artery which has a lower outlet pressure experiences higher velocity values and strain rates due to the pressure imbalance, the wall shear stress near the bifurcation point in this artery is higher than the other. Further, the upper artery has higher shear loading than the bottom one. Although the pressure imbalance has a significant influence on the shear stress distribution in the iliac bifurcations, the wall shear stress at the proximal end of the aneurysm does not seem to be affected. Due to the effect of imbalance outlet pressure, when the flow accelerates, the distal end of the aneurysm tends to experience higher (24.5%) WSS. Therefore, the imbalance pressure effect can not be neglected for wall shear stress analysis in the iliac artery. For specific case with iliac aneurysm, both imbalance outlet pressure and geometrical effect need to be considered.

6.3 Conclusion

The predictions of the pulsatile flow within the AAA bifurcation model show that the Womersley inlet velocity distribution provides for a reasonably accurate description. There are some limitations using the Womersley inlet condition. The Womersley solution is true assuming a constant radius straight tube with rigid wall. However, the real blood vessels are not rigid and with biometric curve. The cross section of the artery is not a perfect circle. The Womersley solution can not 100% represents the real pulsatile velocity profile within the vessel. Using in vivo real velocity measurement as the inlet condition is the best choice. But
it is very expensive and sometime impossible to do the in vivo velocity measurement. Therefore, Womersley condition is an easy and reasonable choice to simulate the inlet boundary condition.

The geometry of the bifurcating region has significant influences on the upstream flow field. Furthermore, stronger secondary flows are observed in the bifurcation zone.

Analysis of the particular rheology models employed in this study shows that the Newtonian model can not provide accurate predictions for hemodynamics in complex geometry such as AAA. The Newtonian model also tends to under predict the wall shear stress as compared with the non-Newtonian model at peak systole. The non-Newtonian properties of the blood appear to provide a stabilizing effect on the flow caused by the higher viscosity (red blood accumulation). The wall shear stress was found to rapidly change near both the proximal and distal sides of the aneurysm during the whole cardiac cycle. This may lead to a higher rupture risk within these regions. At peak systole, peak shear stress was found near the bifurcation point. Therefore, it is important to research the effect of imbalanced pressure outlet.

Results also show that outlet pressure imbalance significantly affects the flow and the shear loading in the iliac arteries. The iliac bifurcation with lower pressure outlet experiences a higher shear loading. However, the pressure imbalance appears to display negligible influence on the upstream flow in the aneurysm. The imbalance outlet pressure can be neglected for the cases with health iliac artery, while it can not be neglected for the cases with iliac aneurysm or stenoses.

The full 3D analysis of AAA has been studied in this chapter, the CFD methods with
suitable viscosity model and boundary conditions can predict the blood flow successfully. 3D transient analyses of total drag to the stent graft are also very important in AAA hemodynamic research. The flow simulation within the stent model using the same CFD methods applied in this chapter will be presented in Appendix E. The influence of geometry to the total forces acting on the stent is studied details in Appendix E.
Chapter 7

Conclusion and Future Work

This thesis is primarily concerned with developing suitable CFD technique for blood flow and stresses simulation in Abdominal Aortic Aneurysm. The wall stresses distribution of the AAA and the hemodynamic are the key factors to be calculated to understand the mechanism of the growth of AAA.

In the first part, in order to improve the accuracy of the fluid solver, a modified OCI (based on the classic OCI) scheme has been originally developed and tested. The modified upwind OCI scheme tends to perform better at high cell Reynolds number while the classical OCI fails to predict acceptable results. The upwind OCI has a wider range of cell Reynolds number applicability compared with the classical OCI scheme. Both the classic and the current OCI schemes have only been applied with rectangular mesh in the current study. The OCI family numeric schemes can be applied to get more accurate results for simple geometry using rectangular grid. This method can be further developed to calculate the FSI problems accompany with Immerse Boundary Methods (IBMs) in the future.

Secondly, a velocity based finite volume method has been developed originally considering the solid and fluid is the same continuum. All classic 1D, 2D and 3D cases have been tested and validated applying this method. The 1D numerical experiments show that this
method gives less temporal numerical damping and less deviation compared with two classic temporal discretization methods. The current method is of second order accuracy in time by comparing the simulation with Jasak and Weller’s (2000) results. High CFL number causes high numerical dissipation, while low CFL number leads to high numerical dispersion. CFL number should be carefully selected for this method in order to improve the accuracy of the calculation and reduce the computational cost. A wide range of geometries and different case parameters are also tested to show the reliability of the solver. The validation shows that the current velocity based method can predict the solid displacement and velocity field correctly. One should notice that the current method does not consider the conservation of area for solid cause the displacement of the tested case is not large. The volume conservation needs to be prior considered in the future study.

In addition, 1D FSI simple piston case is tested to understand the reliability of the method. It is found out that the velocity based method introduces less numerical damping compared to the stagger and the monolithic methods. The key factors of the FSI coupling are also investigated. Both geometric conservation law (GCL) of moving mesh (fluid part) and interaction consistency law (ICL) are important to maintain the accuracy of the computational FSI problems. In addition, second order implicit temporal discretization which reduces the mass accumulation is a better selection for FSI prediction. The simulation also concludes that the velocity based FSI coupling algorithm satisfies the ICL at the boundary and the interface.

Thirdly, finite volume numerical method and Newtonian model have been employed to simulate the steady flow field of the AAA model. Good agreement between numerical prediction and experimental data has been obtained for 2D AAA without iliac bifurcation. It
shows clearly that Fluent could capture both the flow behaviour and wall shear stress and can thereby be extended to pulsatile cases with non-Newtonian viscosity model.

Moreover, pulsatile boundary conditions and non-Newtonian blood viscosity models have been employed to simulate the flow field of 2D AAA model. A comparative analysis of the velocity field near the aneurysm neck has been discussed. A Womersley velocity distribution expression based on the volume flow rate is originally developed to make a better assumption of the inlet boundary condition. It is found that the parabolic boundary condition is not suitable for the velocity calculation when the Womersley number is high. The Newtonian model also tends to under predict the wall shear stress at both proximal and distal end of the AAA as compared with the non-Newtonian model. The current work is helpful to provide a more realistic pulsatile boundary condition (Womersley condition). The Womersley boundary also improves the computational efficiency as compared with the parabolic inlet boundary, cause no additional aneurysm neck calculation domain is needed.

Furthermore, based on the new developed Womersley conditions and the application of the non-Newtonian model, fully three dimensional analysis have been undertaken. The 3D velocity distribution near the aneurysm neck also confirms the importance of using a Womersley like shape inlet boundary. Wall shear stress distribution of the artery wall has been shown during the full cardiac cycle. The wall shear stress was found to rapidly change near both the proximal and distal sides of the aneurysm during the whole cardiac cycle. At peak systole, peak shear stress was found near the bifurcation point. These results are of significance to partially point out the rupture risk location of the aneurysm. The finding of the risk location (peak WSS location) matches some previous clinical researches. The imbalance
iliac bifurcation effect is originally studied by differ the outlet pressure boundary conditions. Results show that outlet pressure imbalance significantly influences the flow and the shear loading in the iliac arteries. The iliac bifurcation with lower pressure outlet experiences a higher shear loading. However, the pressure imbalance appears to a negligible influence on the upstream flow in the aneurysm. The imbalance outlet pressure can be neglected for the cases with health iliac artery, while it can not be neglected for the cases with unhealthy artery such as the arteries with aneurysm and stenoses.

In terms of the stent cases, a total WSS and drag analysis has been conducted with different geometries. The numerical simulations show that the bifurcation angle plays an important role on both the WSS and the total drag. High bifurcation angle set up may increase both the displacement drag and the migration risk. The imbalance effect caused by the iliac artery diameters on the total drag is also significant. The force acting on the bifurcation is of great importance. Stent grafts with larger iliac diameters and/or uniform diameters may decrease the total drag and migration rate.

In the future, since the displacement and stresses analysis can be calculated correctly for 2D/3D cases and the existing 1D FSI algorithm is developed based on Navier-Stokes equations, the velocity based finite volume FSI solver will be extended to calculate 2D, 2D axisymmetric and 3D cases. The volume conservation needs to be built up. Lots of developments need to be done in the future as the current method is not fully complete for 2D and 3D solver. Furthermore, the pulsatile Womersley inlet boundary condition and the non-Newtonian model will be applied to the 3D FSI cases to obtain the fully velocity and stresses fields. Moreover, realistic 3D AAA models captured from patient specific CT/MR
images will be used to simulate the stresses of the aneurysm wall and the total drag of the stent.
Appendix A

Numeric method for upwind OCI scheme

Both the classic and the modified upwind operator compact implicit (OCI) formulas are derived in this section for uniform and non-uniform grids.

Considered the basic convection diffusion difference equation:

$$ L(u) = \frac{\partial u}{\partial t} = a(x) \frac{\partial^2 u}{\partial x^2} + b(x) \frac{\partial u}{\partial x} \quad (A1) $$

Assuming a linear relationship between $u$ and $L(u)$ at the local point in the follow form:

$$ r^{-} u_{i-1} + r^{0} u_{i} + r^{+} u_{i+1} = q^{-} L(u)_{i-k_{-}} + q^{0} L(u)_{i} + q^{+} L(u)_{i+k_{+}} \quad (A2) $$

where $0 < |k_{-}|, |k_{+}| \leq 1$. Using Taylor’s series expansion at the point $i$, the values $u_{i-1}$, $u_{i+1}$, $L(u)_{i-k_{-}}$ and $L(u)_{i+k_{+}}$ can be expressed as

$$ u_{i-1} = u_{x-\Delta x_{-}} = u_{x} - \Delta x_{-} \frac{\partial u}{\partial x} + \frac{(\Delta x_{-})^2}{2!} \frac{\partial^2 u}{\partial x^2} - \frac{(\Delta x_{-})^3}{3!} \frac{\partial^3 u}{\partial x^3} + \frac{(\Delta x_{-})^4}{4!} \frac{\partial^4 u}{\partial x^4} \ldots (A3) $$

$$ u_{i+1} = u_{x+\Delta x_{+}} = u_{x} + \Delta x_{+} \frac{\partial u}{\partial x} + \frac{(\Delta x_{+})^2}{2!} \frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x_{+})^3}{3!} \frac{\partial^3 u}{\partial x^3} + \frac{(\Delta x_{+})^4}{4!} \frac{\partial^4 u}{\partial x^4} \ldots (A4) $$

$$ L(u)_{i-k} = L(u)_{x-k_{-} \Delta x_{-}} = a(x-k_{-}\Delta x_{-}) \frac{\partial^2 u}{\partial x^2} + b(x-k_{-}\Delta x_{-}) \frac{\partial u}{\partial x} \quad (A5) $$

$$ + \frac{(k_{-}\Delta x_{-})^2}{2!} (a(x-k_{-}\Delta x_{-}) - k_{-}\Delta x_{-} b(x-k_{-}\Delta x_{-})) \frac{\partial^3 u}{\partial x^3} $$

$$ + \frac{(k_{-}\Delta x_{-})^3}{3!} (a(x-k_{-}\Delta x_{-}) - k_{-}\Delta x_{-} b(x-k_{-}\Delta x_{-})) \frac{\partial^4 u}{\partial x^4} + \ldots $$
\[ L(u)_{i\rightarrow k} = L(u)_{x+k_i\Delta x_i} = a(x+k_i\Delta x_i) \frac{\partial^2 u}{\partial x^2} + b(x+k_i\Delta x_i) \frac{\partial u}{\partial x} + b(x+k_i\Delta x_i) \frac{\partial^2 u}{\partial x^2} \]
\[ = b(x+k_i\Delta x_i) \frac{\partial u}{\partial x} + (a(x+k_i\Delta x_i) + k_i\Delta x_i b(x+k_i\Delta x_i)) \frac{\partial^2 u}{\partial x^2} + (k_i\Delta x_i) \frac{\partial^3 u}{\partial x^3} + \frac{(k_i\Delta x_i)^2}{2!}(a(x+k_i\Delta x_i) + k_i\Delta x_i b(x+k_i\Delta x_i)) \]
\[ + \frac{k_i\Delta x_i}{3} b(x+k_i\Delta x_i) \frac{\partial^4 u}{\partial x^4} + \ldots \]

Multiplying (A3)-(A6) by \( \alpha, \beta, \gamma \) and \( \delta \), respectively, it can obtain the following relation

\[ \alpha u_{i+1} + \beta u_{i-1} + \gamma L(u)_{i-k_i} + \delta L(u)_{i+k_i} \]
\[ = (\alpha + \beta)u_i + \overline{B} \frac{\partial u}{\partial x_i} + \overline{A} \frac{\partial^2 u}{\partial x_i^2} + \overline{C} \frac{\partial^3 u}{\partial x_i^3} + \overline{D} \frac{\partial^4 u}{\partial x_i^4} + \text{TruncationError} \]

or

\[ \alpha u_{i+1} + \beta u_{i-1} - (\alpha + \beta)u_i = -\gamma L(u)_{i-k_i} - \delta L(u)_{i+k_i} \]
\[ + \overline{B} \frac{\partial u}{\partial x_i} + \overline{A} \frac{\partial^2 u}{\partial x_i^2} + \overline{C} \frac{\partial^3 u}{\partial x_i^3} + \overline{D} \frac{\partial^4 u}{\partial x_i^4} + \text{TruncationError} \]

In order to obtain (A7), the coefficients of the derivative should be has the following form:

\[ \overline{B} = \alpha \Delta x_+ - \beta \Delta x_- + \gamma b(x-k_i\Delta x_-) + \delta b(x+k_i\Delta x_+) = b(x) \]
\[ \overline{A} = \alpha \Delta x_+^2 - \beta \Delta x_-^2 + \gamma (a(x-k_i\Delta x_-) - k_i\Delta x_- b(x-k_i\Delta x_-)) + \delta (a(x+k_i\Delta x_+) + k_i\Delta x_+ b(x+k_i\Delta x_+)) = a(x) \]
\[ \overline{C} = \alpha \Delta x_+^3 - \beta \Delta x_-^3 - \gamma k_i\Delta x_-(a(x-k_i\Delta x_-) - \frac{k_i\Delta x_-}{2} b(x-k_i\Delta x_-)) + \delta k_i\Delta x_+ (a(x+k_i\Delta x_+) + \frac{k_i\Delta x_+}{2} b(x+k_i\Delta x_+)) = 0 \]
\[ \overline{D} = \alpha \Delta x_+^4 - \beta \Delta x_-^4 + \gamma (k_i\Delta x_+)^2 (a(x-k_i\Delta x_-) - \frac{k_i\Delta x_-}{3} b(x-k_i\Delta x_-)) + \delta \frac{(k_i\Delta x_+)^2}{2} (a(x+k_i\Delta x_+) + \frac{k_i\Delta x_+}{3} b(x+k_i\Delta x_+)) = 0 \]

This can also be expressed as
Let \( D \) be the determinant of the matrix on the left hand side of \( A_{10} \), then

\[
\left[ \begin{array}{ccc}
\Delta x_+ & -\Delta x_- & b(x-k\Delta x_-) \\
\Delta x_-^2 & \frac{\Delta x_-^2}{2} & a(x-k\Delta x_-) \\
\Delta x_- & \frac{\Delta x_-}{2} & -k\Delta x_- b(x-\Delta x_-) \\
\Delta x_-^3 & \frac{\Delta x_-^3}{3!} & -k\Delta x_- (a(x-k\Delta x_-)) \\
\Delta x_-^4 & \frac{\Delta x_-^4}{4!} & \left(\frac{\Delta x_-^2}{2}\right) (a(x-k\Delta x_-)) \\
\end{array} \right]
\]

which means only the left \( L(u) \) value are considered, \( A_{10} \) can be further simplified as

\[
\left[ \begin{array}{ccc}
\Delta x_+ & -\Delta x_- & b(x-k\Delta x_-) \\
\Delta x_-^2 & \frac{\Delta x_-^2}{2} & a(x-k\Delta x_-) \\
\Delta x_- & \frac{\Delta x_-}{2} & -k\Delta x_- b(x-\Delta x_-) \\
\Delta x_-^3 & \frac{\Delta x_-^3}{3!} & -k\Delta x_- (a(x-k\Delta x_-)) \\
\Delta x_-^4 & \frac{\Delta x_-^4}{4!} & \left(\frac{\Delta x_-^2}{2}\right) (a(x-k\Delta x_-)) \\
\end{array} \right]\cdot \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} = \begin{bmatrix} b(x) \\ a(x) \\ 0 \\ 0 \end{bmatrix} \quad (A_{10})
\]

Let \( D \) is the determinant of the matrix on the left hand side of \( A_{10} \), then

\[
D = \left( 12a_{a_{i+j}}(k-1)(\Delta x_+^2 - \Delta x_-^2 + \Delta x_+ \Delta x_- + 4k\Delta x_+^2 + 2k\Delta x_+ \Delta x_-) \\
-2a_{b_{i+j}} \Delta x_- (8k^3 \Delta x_-^2 + 4k^3 \Delta x_- \Delta x_+ - 15k^2 \Delta x_-^2 - 3k^2 \Delta x_- \Delta x_+ + 3k^2 \Delta x_+^2) \\
+6k\Delta x_-^2 - 6k\Delta x_- \Delta x_+ - 6k\Delta x_-^2 + 3\Delta x_- \Delta x_+ + 2\Delta x_+^2) \\
-2b_{b_{i+j}} \Delta x_- (\Delta x_+ + \Delta x_-) (\Delta x_+ - 2\Delta x_- - 6k\Delta x_- + 3\Delta x_- + 6k\Delta x_+) \\
-b_{b_{i+j}} k\Delta x_-^2 (\Delta x_+ + \Delta x_-) (k-1)(\Delta x_+ + 2k\Delta x_- - 3k\Delta x_- - 4k\Delta x_+) \right)
\]

\[
D\gamma = \left( 12a_{a_{i+j}}(k^2 \Delta x_-^2 + \Delta x_+^2 - \Delta x_- \Delta x_+ - 2k\Delta x_-^2 + 2k\Delta x_- \Delta x_+) \\
+2a_{b_{i+j}} k\Delta x_-^2 (4k^3 \Delta x_-^2 - 4k^3 \Delta x_- \Delta x_+ - 3k^2 \Delta x_-^2 - 3k^2 \Delta x_- \Delta x_+ + 3k^2 \Delta x_+^2) \\
-2b_{b_{i+j}} k\Delta x_- (\Delta x_+ + 3k\Delta x_- - 3k\Delta x_- - 6k\Delta x_+) \\
+k b_{b_{i+j}} k\Delta x_-^2 \Delta x_+ (2\Delta x_+ + 3k\Delta x_- - 3k\Delta x_- - 4k^2 \Delta x_+) \right)
\]
Thus, the values of $Q$ and $R$ become

$$
q^{i-1} = -\gamma D, q^{i+k} = -\delta D, q^0 = D
$$

$$
r^- = D\beta, r^+ = D\alpha, r^0 = -(r^- + r^+)
$$

This can be call modified upwind OCI scheme. Assuming $k = \frac{1}{2}$ and uniform grid $(\Delta x_+ = \Delta x_- = \Delta x)$, (A11-A15) can be further simplified as

$$
D = 48a_ia_{i-1/2} - \Delta x(a_{i-1}b_{i-1/2} + 8b_{i-1}a_{i-1/2}) + \Delta x^2b_{i-1}b_{i-1/2}
$$

$$
D\gamma = -12a_ia_{i-1/2} - \Delta x(a_{i}b_{i-1/2} + 2b_{i}a_{i-1/2}) - \Delta x^2b_{i}b_{i-1/2}
$$

$$
D\delta = 12a_ia_{i-1} - \Delta x(8a_{i}b_{i-1} - 20b_{i}a_{i-1}) - 4\Delta x^2b_{i}b_{i-1}
$$

$$
D\beta2\Delta x^2 = D(2a_0 - \Delta x b_0) - D\delta(2a_{i-1/2} - 2\Delta x b_{i-1/2}) - D\gamma(2a_{i-1} - 3\Delta x b_{i-1})
$$

$$
D\alpha2\Delta x^2 = D(2a_0 + \Delta x b_0) - D\delta2a_{i-1/2} - D\gamma(2a_{i-1} - \Delta x b_{i-1})
$$

The truncation error related to (A7-A9) is given by

$$
\text{Error} = \left[ \frac{a\Delta x^4}{5!} - \frac{b\Delta x^5}{5!} + \frac{\delta(\Delta x)^i}{3!}(a_{i+k} + \frac{k\Delta x}{4}b_{i+k}) - \frac{\gamma(\Delta x)^i}{3!}(a_{i-k} - \frac{k\Delta x}{4}b_{i-k}) \right] \frac{\partial^4 u}{\partial x^4}
$$

(A21)

For small $\Delta x_-$ and $\Delta x_+$, the OCI scheme is seen to be third order accurate.
Appendix B

Figures of 1D linear problem (for Chapter 3)

Fig. B1 Comparison of different numerical schemes for 1D linear problem ($\mu = 0.1$) with 10 nodes uniform grid.

Fig. B2 Comparison of different numerical schemes for 1D linear problem ($\mu = 0.05$) with uniform grid (scale is enlarge for clear view).
Fig. B3 Comparison of different numerical schemes for 1D linear problem ($\mu = 0.01$) with 10 nodes uniform grid.

Fig. B4 Comparison of different numerical schemes for 1D linear problem ($\mu = 0.1$) with 10 nodes non-uniform grid.
Fig. B5 Comparison of different numerical schemes for 1D linear problem ($\mu = 0.05$) with 40 nodes non-uniform grid.

Fig. B6 Comparison of upwind OCI scheme for 1D linear problem ($\mu = 0.002$) between different non-uniform grids.
Figures of 1D non-linear Burger equation (for Chapter 3)

Fig. B7 Comparison of different OCI schemes for 1D Burger equation (μ = 0.5) with uniform grids.

Fig. B8 Comparison of different OCI schemes for 1D Burger equation (μ = 0.03125) with uniform grids.
Fig. B9 Comparison of different OCI schemes for 1D Burger equation (\( \mu = 0.5 \)) with non-uniform grids (20 nodes).

Fig. B10 Comparison of different OCI schemes for 1D Burger equation (\( \mu = 0.0625 \)) with non-uniform grids.
Fig. B11 Comparison of different OCI schemes for 1D Burger equation (\( \mu = 0.0625 \)) with non-uniform grids.

Fig. B12 Comparison of upwind OCI scheme for 1D Burger equation (\( \mu = 0.015625 \)) between different non-uniform grids.
Appendix C

Velocity based finite volume method for Cartesian coordinate

The equilibrium equations of solid in terms of stresses for 3D Cartesian coordinate can be expressed as

\[
\rho \frac{\partial^2 d_x}{\partial t^2} = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} + F_x \tag{C1}
\]

\[
\rho \frac{\partial^2 d_y}{\partial t^2} = \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} + F_y \tag{C2}
\]

\[
\rho \frac{\partial^2 d_z}{\partial t^2} = \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + F_z \tag{C3}
\]

where

\[
\sigma_{xx} = \lambda (e_{xx} + e_{yy} + e_{zz}) + 2\mu e_{xx} \tag{C4}
\]

\[
\sigma_{yy} = \lambda (e_{xx} + e_{yy} + e_{zz}) + 2\mu e_{yy} \tag{C5}
\]

\[
\sigma_{zz} = \lambda (e_{xx} + e_{yy} + e_{zz}) + 2\mu e_{zz} \tag{C6}
\]

\[
\tau_{xy} = 2\mu e_{xy}, \quad \tau_{yz} = 2\mu e_{yz}, \quad \tau_{zx} = 2\mu e_{zx} \tag{C7}
\]

\[
e_{xx} = \frac{\partial d_x}{\partial x}, \quad e_{yy} = \frac{\partial d_y}{\partial y}, \quad e_{zz} = \frac{\partial d_z}{\partial z} \tag{C8}
\]

\[
e_{xy} = \frac{1}{2} \left( \frac{\partial d_x}{\partial y} + \frac{\partial d_y}{\partial x} \right), \quad e_{yz} = \frac{1}{2} \left( \frac{\partial d_y}{\partial z} + \frac{\partial d_z}{\partial y} \right), \quad e_{xz} = \frac{1}{2} \left( \frac{\partial d_z}{\partial x} + \frac{\partial d_x}{\partial z} \right) \tag{C9}
\]

The 3D Cartesian expression of the equilibrium equations (assuming zero body force) can be
obtained in terms of displacement

\[ \rho \frac{\partial^3 d_x}{\partial t^3} = \frac{\partial}{\partial x} \left[ \lambda \left( \frac{\partial d_x}{\partial x} + \frac{\partial d_y}{\partial y} + \frac{\partial d_z}{\partial z} \right) + \mu \left( \frac{\partial d_x}{\partial y} + \frac{\partial d_y}{\partial x} + \frac{\partial d_y}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial d_x}{\partial y} + \frac{\partial d_y}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial d_x}{\partial z} + \frac{\partial d_z}{\partial x} \right) \right] \]

\[ \rho \frac{\partial^3 d_y}{\partial t^3} = \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial d_x}{\partial x} + \frac{\partial d_y}{\partial y} + \frac{\partial d_z}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \lambda \left( \frac{\partial d_y}{\partial x} + \frac{\partial d_y}{\partial y} + \frac{\partial d_y}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial d_y}{\partial z} + \frac{\partial d_z}{\partial y} \right) \right] \]

\[ \rho \frac{\partial^3 d_z}{\partial t^3} = \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial d_x}{\partial x} + \frac{\partial d_z}{\partial y} + \frac{\partial d_z}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial d_y}{\partial x} + \frac{\partial d_z}{\partial y} + \frac{\partial d_z}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left[ \lambda \left( \frac{\partial d_z}{\partial x} + \frac{\partial d_z}{\partial y} + \frac{\partial d_z}{\partial z} \right) \right] \]

Using the displacement-velocity relation

\[ d_i = d_i^{old} + \frac{\Delta t}{2} (u_i^{old} + u_i^{new}), \quad (i = x, y, z) \]

The velocity based equilibrium equations can be calculated as

\[ \frac{\partial u_x}{\partial t} = \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \lambda \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_y}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right) \right] \]

\[ \frac{\partial u_y}{\partial t} = \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \lambda \left( \frac{\partial u_y}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_y}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right) \right] \]

\[ \frac{\partial u_z}{\partial t} = \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial y} + \frac{\partial u_z}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u_z}{\partial x} + \frac{\partial u_z}{\partial y} + \frac{\partial u_z}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left[ \lambda \left( \frac{\partial u_z}{\partial x} + \frac{\partial u_z}{\partial y} + \frac{\partial u_z}{\partial z} \right) \right] \]

The above equations can be discretized using finite volume method by integrating them in the
control volume

\[ \int_{\Omega} \rho \frac{\partial u_i}{\partial t} dV = \rho_p \left( \frac{\partial u_i}{\partial t} \right)_p \Delta x \Delta y \Delta z = \rho_p \frac{u_{i_p}^{new} - u_{i_p}^{old}}{\Delta t} \Delta x \Delta y \Delta z, \quad (i = x, y, z) \quad \text{(C16)} \]

\[ \int_{\Omega} \frac{\partial}{\partial x} \frac{\partial u_i}{\partial x} dV = \left( \frac{\partial u_i}{\partial x} \right)_e - \left( \frac{\partial u_i}{\partial x} \right)_w \Delta y \Delta z, \quad (i = x, y, z) \quad \text{(C17)} \]

\[ \int_{\Omega} \frac{\partial}{\partial y} \frac{\partial u_i}{\partial y} dV = \left( \frac{\partial u_i}{\partial y} \right)_n - \left( \frac{\partial u_i}{\partial y} \right)_s \Delta x \Delta z, \quad (i = x, y, z) \quad \text{(C18)} \]

\[ \int_{\Omega} \frac{\partial}{\partial z} \frac{\partial u_i}{\partial z} dV = \left( \frac{\partial u_i}{\partial z} \right)_f - \left( \frac{\partial u_i}{\partial z} \right)_b \Delta x \Delta y, \quad (i = x, y, z) \quad \text{(C19)} \]

\[ \int_{\Omega} \frac{\partial u_i}{\partial x} dV = [u_{ie} - u_{iw}] \Delta y \Delta z, \quad (i = x, y, z) \quad \text{(C20)} \]

\[ \int_{\Omega} \frac{\partial u_i}{\partial y} dV = [u_{in} - u_{is}] \Delta x \Delta z, \quad (i = x, y, z) \quad \text{(C21)} \]

\[ \int_{\Omega} \frac{\partial u_i}{\partial z} dV = [u_{if} - u_{ib}] \Delta x \Delta y, \quad (i = x, y, z) \quad \text{(C22)} \]

where \( P \) denotes the local point value, \( e, w, n, s, f \) and \( b \) mean the values at the east, west, north, south, front and back surfaces of the control volume. Other source terms can be integrated in similar method. These integrations will lead to a set of linear equations as

\[ \sum_j A_{ij} u_i = \text{source}_j, \quad (j = W, E, N, S, F, B; i = x, y, z) \quad \text{(C23)} \]

**Velocity based finite volume method for 2D cylindrical coordinate**

The equilibrium equations of solid in terms of stresses for 3D cylindrical coordinate can be expressed as

\[ \rho \frac{\partial^2 r}{\partial t^2} = \frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \tau_{r\theta}}{\partial \theta} + \frac{\partial \tau_{rz}}{\partial z} + \frac{1}{r} \left( \sigma_{r\theta} - \sigma_{\theta\theta} \right) + F_r \quad \text{(C24)} \]

\[ \rho \frac{\partial^2 \theta}{\partial t^2} = \frac{\partial \tau_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{\partial \tau_{\theta z}}{\partial z} + \frac{2}{r} \tau_{r\theta} + F_\theta \quad \text{(C25)} \]
\[
\rho \frac{\partial^2 d_i}{\partial t^2} = \frac{\partial \tau_{r_i}}{\partial r} + \frac{1}{r} \frac{\partial \tau_{\theta_i}}{\partial \theta} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{1}{r} \tau_{rz} + F_i
\]  
(C26)

where

\[
\sigma_{rr} = \lambda \left( e_{rr} + e_{\theta\theta} + e_{zz} \right) + 2\mu e_{rr}
\]  
(C27)

\[
\sigma_{\theta\theta} = \lambda \left( e_{rr} + e_{\theta\theta} + e_{zz} \right) + 2\mu e_{\theta\theta}
\]  
(C28)

\[
\sigma_{zz} = \lambda \left( e_{rr} + e_{\theta\theta} + e_{zz} \right) + 2\mu e_{zz}
\]  
(C29)

\[
\tau_{r\theta} = 2\mu e_{r\theta}, \quad \tau_{\theta z} = 2\mu e_{\theta z}, \quad \tau_{rz} = 2\mu e_{rz}
\]  
(C30)

and

\[
e_{rr} = \frac{\partial d_r}{\partial r}, \quad e_{\theta\theta} = \frac{1}{r} \left( d_r + \frac{\partial d_{\theta}}{\partial \theta} \right), \quad e_{zz} = \frac{\partial d_z}{\partial z}
\]  
(C31)

\[
e_{r\theta} = \frac{1}{2} \left( \frac{\partial d_r}{\partial \theta} + \frac{\partial d_{\theta}}{\partial r} - \frac{d_{\theta}}{r} \right)
\]  
(C32)

\[
e_{\theta z} = \frac{1}{2} \left( \frac{\partial d_{\theta}}{\partial z} + \frac{r}{\partial \theta} \right)
\]  
(C33)

\[
e_{z\theta} = \frac{1}{2} \left( \frac{\partial d_z}{\partial \theta} + \frac{\partial d_{r}}{\partial z} \right)
\]  
(C34)

Assuming the geometry is axisymmetric then

\[
d_{\theta} = 0, \quad \frac{\partial d_{\theta}}{\partial \theta} = 0
\]  
(C35)

The 2D cylindrical expression of the equilibrium equations (assuming zero body force) can be obtained

\[
\rho \frac{\partial^2 d_r}{\partial t^2} = \frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{1}{r} \left( \sigma_{rr} - \sigma_{\theta\theta} \right)
\]  
(C36)

\[
\rho \frac{\partial^2 d_z}{\partial t^2} = \frac{\partial \tau_{rz}}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{1}{r} \tau_{rz}
\]  
(C37)

In terms of displacement \( d_i (i = r, \theta, z) \)
\[
\frac{\partial^2 d_i}{\partial t^2} = \frac{\partial}{\partial r} \left[ \lambda \left( \frac{\partial d_i}{\partial r} + \frac{1}{r} d_i + \frac{\partial d_i}{\partial \theta} \right) + 2\mu \left( \frac{\partial d_i}{\partial \theta} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial d_i}{\partial \theta} + \frac{\partial d_i}{\partial z} \right) \right] + \frac{1}{r} \left( 2\mu \frac{\partial d_i}{\partial r} - 2\mu \frac{d_i}{r} \right) \quad (C38)
\]

\[
\frac{\partial^2 d_i}{\partial t^2} = \frac{\partial}{\partial r} \left[ \mu \left( \frac{\partial d_i}{\partial r} + \frac{1}{r} d_i + \frac{\partial d_i}{\partial \theta} \right) \right] + \frac{\partial}{\partial z} \left[ \lambda \left( \frac{\partial d_i}{\partial \theta} + \frac{1}{r} d_i + \frac{\partial d_i}{\partial z} \right) + 2\mu \frac{\partial d_i}{\partial z} \right] + \frac{1}{r} \left( 2\mu \frac{\partial d_i}{\partial \theta} \right) \quad (C39)
\]

Using the displacement-velocity relation 
\[ d_i = d_i^{old} + \frac{\Delta t}{2} (u_i^{old} + u_i^{new}), (i = r, \theta, z) \]

The velocity based equilibrium equations can be calculated as
\[
\rho \frac{\partial u_i}{\partial t} = \frac{\partial}{\partial r} \left[ \lambda \left( \frac{\partial u_i}{\partial r} + \frac{1}{r} u_i + \frac{\partial u_i}{\partial \theta} \right) + 2\mu \frac{\partial u_i}{\partial \theta} \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u_i}{\partial \theta} + \frac{\partial u_i}{\partial z} \right) \right] + \frac{1}{r} \left( 2\mu \frac{\partial u_i}{\partial r} - 2\mu \frac{u_i}{r} \right) \quad (C40)
\]

\[
\rho \frac{\partial u_i}{\partial t} = \frac{\partial}{\partial r} \left[ \mu \left( \frac{\partial u_i}{\partial r} + \frac{1}{r} u_i + \frac{\partial u_i}{\partial \theta} \right) \right] + \frac{\partial}{\partial z} \left[ \lambda \left( \frac{\partial u_i}{\partial \theta} + \frac{1}{r} u_i + \frac{\partial u_i}{\partial z} \right) + 2\mu \frac{\partial u_i}{\partial z} \right] + \frac{1}{r} \left( 2\mu \frac{\partial u_i}{\partial \theta} \right) \quad (C41)
\]

The above equations can be discretized using finite volume method mention in the previous section. The only difference is the boundary condition at r=0.

\[ \text{at } r = 0, \quad \frac{\partial u_i}{\partial r} = 0 \text{ and } \frac{\partial d_i}{\partial r} = 0 \quad (i = r, \theta, z) \quad (C42) \]
Appendix D

List of codes and their function

Boundary conditions codes

“blood_inlet.f90” and “boundary.c”

In Chapter 3 and 4, a piece of Fortran code “blood_inlet.f90” is developed to obtain n=0,1,2,...,24 coefficients in equation 3-10, 3-11 and 3-12 from Fig. 3-1. A user define function (UDF) code “boundary.c” written in C++ is used to input the pulsatile boundary conditions in Fluent. The UDF contains some Bessel function calculation subroutine.

Package of OCI codes

The package of OCI codes mainly contains 19 Fortran source files. They are listed as follow

<table>
<thead>
<tr>
<th>Code</th>
<th>Function Description</th>
</tr>
</thead>
<tbody>
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<td>Header.f90</td>
<td>header of the code to define global variables</td>
</tr>
<tr>
<td>Scheme.f90</td>
<td>main function of the OCI schemes</td>
</tr>
<tr>
<td>Init.f90</td>
<td>function to initial the cases</td>
</tr>
<tr>
<td>Init_cavity.f90</td>
<td>function to initial the 2D shear driven cavity</td>
</tr>
<tr>
<td>Initb.f90</td>
<td>function to initial the boundary conditions</td>
</tr>
<tr>
<td>Grib.f90</td>
<td>function to generate grid</td>
</tr>
<tr>
<td>Grib_cavity.f90</td>
<td>function to generate 2D cavity grid</td>
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<tr>
<td>File</td>
<td>Description</td>
</tr>
<tr>
<td>------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Burger.f90</td>
<td>function to solve Burger’s equation and 1D cases</td>
</tr>
<tr>
<td>Cal_cavity.f90</td>
<td>function to solve steady and unsteady 2D shear driven cavity</td>
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<tr>
<td>Oci_co.f90</td>
<td>function to calculate the OCI coefficients</td>
</tr>
<tr>
<td>Cal_u.f90</td>
<td>function to solve x-momentum equation</td>
</tr>
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<td>Cal_v.f90</td>
<td>function to solve y-momentum equation</td>
</tr>
<tr>
<td>Cal_p.f90</td>
<td>function to couple the pressure using SIMPLE, SIMPLEX, SIMPLER and PISO</td>
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<tr>
<td>Cal.f90</td>
<td>function to calculate additional source terms</td>
</tr>
<tr>
<td>P_solver.f90</td>
<td>function to solve the pressure matrix</td>
</tr>
<tr>
<td>TDMA_solver.f90</td>
<td>function of TDMA solver</td>
</tr>
<tr>
<td>Multi_matrix.f90</td>
<td>function of matrixes multiplication</td>
</tr>
<tr>
<td>Tridiagonal_matrix_inversion.f90</td>
<td>function of tri-diagonal matrix inversion</td>
</tr>
<tr>
<td>Cavity_inout.f90</td>
<td>functions to input and output the cavity results</td>
</tr>
</tbody>
</table>
**Package of velocity based finite volume method codes.**

The package for 2D and 3D solid and 1D FSI piston codes mainly contain 6 Fortran files. They are listed as follow:

- **CFD_win.f95**: main function of the velocity based finite volume method
- **OneD_FSI.f95**: subroutine to solve the 1D FSI piston problems
- **Grid.f95**: function to generate grid
- **Rectangular_Grid.f95**: function to generate 2D and 3D rectangular grid
- **Solver.f95**: subroutine contains functions of matrix solver. It includes TDMA solver, solvers using Jacobi method, solvers using point Jacobi method, solvers using point Gauss-Seidel method, solvers using line Gauss-Seidel method, solvers using ADI method, solvers using SIP method, solvers using projection method, solvers using minimal residual method and solvers using residual norm method
- **FV_solid.f95**: main subroutine using velocity based finite volume method to solve 2D and 3D solid.
It includes function to initial the cases, function to generate meshes, function to solve x-momentum equation, function to solve y-momentum equation, function to solve z-momentum equation, function to couple the pressure using SIMPLE, SIMPLEC, SIMPLER and PISO algorithms, main function to solve steady and unsteady 2D and 3D solid, functions to input and output the cavity results.
Appendix E

Transient Analysis of Stresses of Bypass Stent Graft

E.1 Bifurcated stents models

In order to understand the full 3D hemodynamic effects on the stent behaviour, simple stent models with different bifurcation angles are investigated. These models are defined by the main aortic and the iliac artery diameters, including their lengths and the bifurcation angle. The main aortic diameter of the stent is set to be 24mm and the length is assumed to be 180mm. Different bifurcation angles (15°, 25°, 30°, 35°, 45°) are employed. The iliac diameters (left and right) and length are defined to be 16mm and 80mm for the above models. The imbalance effect of the iliac arteries is also investigated for the 30° case. Different iliac diameters (left iliac: 16mm and right iliac: 15mm and 15.5mm) are applied for these cases.

The parameters of different cases are list in table E-1.

<table>
<thead>
<tr>
<th>Cases Parameters</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bifurcation angles</td>
<td>15°</td>
<td>25°</td>
<td>30°</td>
<td>35°</td>
<td>45°</td>
<td>30°</td>
<td>30°</td>
</tr>
<tr>
<td>Left iliac diameter</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
</tr>
<tr>
<td>Right iliac diameter</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>16mm</td>
<td>15.5mm</td>
<td>15mm</td>
</tr>
</tbody>
</table>

Table. E-1 Geometrical parameters for different stent cases.
Fig. E-1 3D Abdominal aortic stent graft model.

E.2 Shear stress and total drag analysis amongst different abdominal aortic stent models with bifurcation

Stent migration is very important in EVAR. Stent migration takes place when the total drag introduced on the stent graft exceeds the limit stent displacement force (Martin et al., 1998; Benjamin et al., 2007). In order to understand the total drag imposed on the stent graft, the full 3D velocity and the accompanying pressure fields must be computed. Once the velocity and pressure fields are calculated, the total drag of the stent graft can be described by following expression using simple fluid dynamic formulation:

\[
\text{total drag} = \text{total wall shear stress} + \text{pressure force} \quad (E-1)
\]

where the total wall shear stress is the integrated WSS for the whole stent and the pressure force can be expressed as

\[
\text{pressure force} = \text{stent inlet pressure} \times \text{stent inlet area} - \sum \text{stent outlet pressure} \times \text{stent outlet area} \times \cos \phi \quad (E-2)
\]
where $\phi$ is the angle between the inlet and the outlet.

As pointed out in the above section and in previous research (Ma and Turan, 2011), the boundary conditions affect the flow field significantly. Fig. E-2 and E-3 depict the influence of boundary conditions and the viscous models regarding the integrity of the stress field. It can be seen that the maximum stress and the stress differences due to boundary conditions occur at the peak systole, a behaviour validated by previous research (Khanafer et al, 2006, Ma and Turan, 2011). The viscous models used affect the WSS directly according to Fig. 6-15 by 14.0%, while the inlet boundary conditions modify the total drag according to Fig. E-2 at 3.5% difference at the peak systole. The results for the total drag also agree with Howell et al’s (2007) both in terms of qualitative and quantitative behaviour.

Fig. E-2 Total WSS of the stent in a cardiac cycle with different boundary conditions (30 degree bifurcation angle).
Many previous studies indicated that the geometry of the stent, especially the bifurcation angle is crucially important in reading the stent stress levels (Li and Kleinstreuer, 2007, Ma and Turan, 2011). The author also tested this geometry influence using five different bifurcation angles (15°, 25°, 30°, 35°, 45°). Fig. E-4 and Fig. E-5 illustrate the stress differences for different geometries. Greater WSS occur with lower bifurcation angle around the peak systole, while the WSS does not display any differences for the rest of the cardiac cycle. The WSS difference is 38.7% for bifurcation angles of 15° and 45°. However, the bifurcation angle significantly affects the total drag with the higher bifurcation angle imposing greater total drag. This is primarily caused by the turning effect experienced by the blood in the stent, i.e. greater total force is needed to turn the flow through higher angles. This also means that the stent with higher bifurcation angle may have a higher migration risk, pointing to the benefits of an extended study regarding flow induced force at the bifurcation point (Howell et al.,
Fig. E-4 Total WSS of the stent in a cardiac cycle with different bifurcation angles (Womersley inlet and non-Newtonian model).

Fig. E-5 Total drag of the stent in a cardiac cycle with different bifurcation angles (Womersley inlet and non-Newtonian model).
Size effect is another crucial factor regarding stent migration. Previous CFD simulation (Howell et al., 2007) indicated that the size of the trunk of the stent graft directly influence the migration rate. This research mainly focuses on the iliac diameter and its imbalance effect on the total stress levels. With the same bifurcation angle, stents with uniform iliac diameters (16mm for both iliac arteries) and different diameters (16mm for the left iliac artery and 15.5mm/15mm right iliac artery) are tested (Fig. E-6 and E-7). The stent with the narrower iliac diameter experiences higher WSS and total drag. This indicates that the narrow ends of the stent graft may cause a higher migration risk. All these findings are expected to provide the stent manufacturers with a rationally based design procedure for optimum stent geometry.

Fig. E-6 Total WSS of the stent in a cardiac cycle with different iliac artery size (Womersley inlet and non-Newtonian model with 30° bifurcation angle).
Fig. E-7 Total drag of the stent in a cardiac cycle with different iliac artery size (Womersley inlet and non-Newtonian model with 30° bifurcation angle).

For stent-graft force balance analysis, the numerical simulations show that the bifurcation angle plays an important role regarding the WSS as well as the total drag. High bifurcation angle set up may increase both the displacement drag and the migration risk. The imbalance effect caused by the iliac artery diameters on the total drag is also significant. The force acting on the bifurcation is of great importance. Stent grafts with larger iliac diameters and/or uniform diameters may decrease the total drag and migration rate.

With the use of practical inlet condition based on the Womersley theory and non-Newtonian model, predictions may be obtained to help improve understanding of the flow field and the growth mechanism of AAAs. The numerical simulation with suitable geometry and boundary conditions can also help improve the design of the stent. The limitations on this research are the rigid wall assumption, since the blood vessel is compliant rather than rigid. The sac pressure may also influence the migration risk. Therefore, future
work will focus on the fluid-structure interaction predictions of 3D AAA bifurcating model for the particular stent design using more accurate boundary conditions. The next chapter is going to present a high order numerical scheme which aims to provide accurate results in general CFD application.
Appendix F

Abstracts of Journal Papers

In this appendix, the titles and abstracts of journal papers published/submitted during the PhD research are provided.

Pulsatile non-Newtonian haemodynamics in a 3D bifurcating abdominal aortic aneurysm model

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(Received 2 November 2009; final version received 12 May 2010)

Numerical prediction of non-Newtonian blood flow in a 3D abdominal aortic aneurysm bifurcating model is carried out. The non-Newtonian Carreau model is used to characterise the shear thinning behaviour of the human blood. A physical inlet velocity waveform incorporating a radial velocity distribution reasonably representative of a practical case configuration is employed. Case studies subject to both equal and unequal outlet pressures at iliac bifurcations are presented to display convincingly the downstream pressure influences on the flow behaviour within the aneurysm. Simulations indicate that the non-Newtonian aspects of the blood cannot at all be neglected or given a cursory treatment. The wall shear stress (WSS) is found to change significantly at both the proximal and distal ends of the aneurysm. At the peak systole, the WSS is peak around the bifurcation point, whereas the WSS becomes zero in the bifurcation point. Differential downstream pressure fields display significant effects regarding the flow evolution in the iliac arteries, whereas little or no effects are observed directly on the flow details in the aneurysm.

Keywords: abdominal aortic aneurysm; pulsatile; computational fluid dynamics; wall shear stress
Analysis of Non-Newtonian Blood Flow in an Abdominal Aortic Aneurysm and Bifurcated Stents Incorporating Womersley Number to Characterize the Inlet Velocity Distribution

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Abstract

Non-Newtonian blood flow in a two-dimensional abdominal aortic aneurysm (AAA) model and three-dimensional stent designs are investigated by solving the Navier-Stokes equations coupled with the Carreau model, which represents the shear thinning behaviour of the human blood. Physical inlet velocity distribution as well as a realistic outlet pressure variation is applied to simulate realistic boundary conditions. Additionally, an improved pulsatile velocity distribution based on the Womersley theory vis-à-vis the parabolic shape velocity profile is introduced. Results indicate that the velocity distribution based on the Womersley theory represents the pulsatile flow behaviour in a more realistic manner as compared to the parabolic velocity profile. Flow fields and wall shear stresses are investigated using both Newtonian and non-Newtonian models. The non-Newtonian viscous properties affect the flow field significantly. Total drag is studied with a view to optimizing for different three-dimensional stent models.

Note that this paper was submitted to Computer Method of Biomechanics and Biomedical Engineering

A velocity-based fluid-structure interaction algorithm and its application to the piston problem

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Abstract

A finite volume velocity-based time marching fluid-structure interaction (FSI) algorithm is developed and investigated. The FSI piston problem is studied to understand the feasibility and accuracy of the coupling algorithms. First, an investigation of one dimension wave equation is presented in order to test the performance of the velocity-based time marching method for solid. This method shows less numerical damping compared with some classic implicit transition methods. This method is also tested with two-dimensional and three-dimensional cases. The results show good agreement with some analytical solution. A velocity-based FSI coupling algorithm is then introduced in order to reduce the numerical damping for FSI problems. This method considers both fluid and structure as a single phase, thus only one set of velocity-based momentum equations is calculated. This algorithm avoids additional boundary conditions transfer between the fluid and solid interface. Linear acoustic as well as nonlinear Euler equations for compressible fluid mechanic are investigated. The velocity-based algorithm shows less numerical damping on the FSI piston problem compared with the monolithic FSI schemes. This method also shows good replicability and feasibility for two-dimension and three-dimension solvers.

Note that this paper was submitted to Journal of Computers and Structure.
Bibliography


Technology 30, 283-297.


Flow Computations on Moving Grids, AIAA journal, 1030-1037.


in Abdominal Aortic Aneurysms: Effects of Asymmetry and Wall Thickness. Biomedical Engineering Online 4:64.


