UNIVERSITI PUTRA MALAYSIA

DEVELOPMENT OF NON-BOUNDARY-FITTED CARTESIAN GRID METHOD FOR NUMERICAL SIMULATION OF MECHANICAL HEART VALVE AND THE POTENTIAL FOR BLOOD CLOTTING

MOHAMAD SHUKRI BIN ZAKARIA

FK 2018 95
DEVELOPMENT OF NON-BOUNDARY-FITTED CARTESIAN GRID METHOD FOR NUMERICAL SIMULATION OF MECHANICAL HEART VALVE AND THE POTENTIAL FOR BLOOD CLOTTING

By

MOHAMAD SHUKRI BIN ZAKARIA

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

April 2018
COPYRIGHT

All material contained within the thesis, including without limitation text, logos, icons, photographs and all other artwork, is copyright material of Universiti Putra Malaysia unless otherwise stated. Use may be made of any material contained within the thesis for non-commercial purposes from the copyright holder. Commercial use of material may only be made with the express, prior, written permission of Universiti Putra Malaysia.

Copyright ©Universiti Putra Malaysia
Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

DEVELOPMENT OF NON-BOUNDARY-FITTED CARTESIAN GRID METHOD FOR NUMERICAL SIMULATION OF MECHANICAL HEART VALVE AND THE POTENTIAL FOR BLOOD CLOTTING

By

MOHAMAD SHUKRI BIN ZAKARIA

April 2018

Chairman : Kamarul Arifin bin Ahmad, PhD
Faculty : Engineering

Computational fluid dynamics (CFD) simulations are becoming a reliable tool in understanding disease progression, investigating blood flow patterns and evaluating medical device performance such as mechanical heart valves (MHV). Previous studies indicated that the non-physiological flow pattern (i.e. recirculation, stagnation, and vortex) might cause a trapped platelet and be responsible for the formation of blood clots in MHV. Accurate simulation of this flow requires a high order accuracy numerical scheme together with a scale resolving turbulence model such as large eddy simulation (LES). This requires the use of uniform orthogonal grids for the discretisation process, which is not able to handle complex branching arterial domains that contain MHV, where the generation are usually boundary-fitted (BF) grid with non-orthogonality and distortions. Therefore, non-boundary fitted (NBF) Cartesian grid method is an alternative solution. The objective of this study is to develop a new NBF method based on the volume of fluid (VOF), containing the colour function, namely NBF-VOF Cartesian grid method. A single set of governing equation is used for both solid and fluids identified by unity colour function and zero colour function respectively. The solid was treated as a fluid with very high viscosity to theoretically reduce its deformability, and subsequently satisfy a no-slip condition at the boundary. In the first attempt, we found that in prior, the treatment was not satisfied. To suppress the fluid velocities in the solid, we introduced the artificial term derived from the colour function into an algebraic system of momentum equations, which had a significant impact on the originality of this study. The developed solver, NBF-VOF, is then thoroughly validated using a variety of numerical and experimental results available in the literature which is Hagen-Poiseuille flow, lid-driven cavity, flow over a cylinder, $90^\circ$ tube flow, and pulsatile flow through the real anatomic aorta. Opensource CFD software was used as our simulation platform. Although the second order method degenerates the spatial accuracy of convergence rate as function of the grid size from 2 to 1.5, an agreement was found for all cases qualitative and quantitatively. The grid uncertainty obtained was
less than 5%, which was within the acceptable range. The computational time was lower when the viscosity of solid was higher. However, higher solid viscosity gives lagging in the result for transient cases. Despite this, using higher time step, until the maximum Courant number of 4.0, can speed up the simulation time and preserved the stability. Finally, another breakthrough in this study was the application of the solver to simulate pulsatile blood flow of MHV placed in an axisymmetric and real patient anatomic aorta with the sinus, which reveals complex blood flow patterns, shear stress loading, and history of particles age in the local domain, that consequently can identified the potential of blood clotting.
Pembangunan kaedah grid-tidak-terikat untuk simulasi berangka pada injap jantung mekanikal dan potensi untuk pembekuan darah

Oleh

Mohamad Shukri bin Zakaria

April 2018

Pengerusi: Kamarul Arifin bin Ahmad, PhD
Fakulti: Kejuruteraan

Pengkomputeran dinamik bendalir (CFD) telah menjadi alat yang boleh dipercayai dalam memahami perkembangan penyakit, menyiasat corak aliran darah dan menilai prestasi peranti perubatan seperti injap jantung mekanikal (MHV). Kajian terdahulu menunjukkan bahawa corak aliran bukan fisiologi, menyebabkan platelet terperangkap, bertanggung-jawab ke atas pembentukan darah beku pada MHV. Ketepatan simulasi aliran ini memerlukan darjah ketepatan yang tinggi dengan skala yang dapat menyelesaikan masalah segregasi simula eddy besar (LES). Ini memerlukan penggunaan grid ortogonal seragam, yang tidak dapat dikendalikan oleh bentuk arteri yang kompleks yang menganungi MHV, di mana grid biasanya digunakan adalah kaedah grid terikat (BF) yang tidak ortogonal dan terherot. Oleh itu, kaedah grid tidak terikat (NBF) adalah penyelesaian alternatif. Objektif kajian ini adalah untuk membangunkan kaedah NBF baru berdasarkan jumlah cecair (VOF) yang mengandungi warna berfungsi diberi nama NBF-VOF. Satu persamaan digunakan untuk mengenal keadaan dua pepejal dan bendalir adalah melalui warna fungsi uniti dan kosong. Pepejal dianggap sebagai bendalir dengan kelikatan yang sangat tinggi yang secara teorinya mengurangkan perubahan bentuk, dan memenuhi syarat tidak-slip di sempadan. Pada percubaan awal, kami dapatkan bahawa, kaedah itu tidak memuaskan. Untuk terus menyekat aliran bendalir dalam pepejal, kami memperkenalkan istilah buatan yang diterbitkan dari warna fungsi ke dalam sistem algebra persamaan momentum. Seterusnya, kaedah NBF-VOF disahkan menggunakan pelbagai hasil kaedah berangka dan eksperimen yang terdapat dalam literatur melalui perisian sumber terbuka OpenFoam. Aliran Hegen-poissuelle, rongga yang didorong, aliran ke atas silinder, 90° aliran tiub, dan aliran denyutan melalui aorta anatomi sebenar. Kesamaan yang sangat baik telah dihasilkan untuk semua kes. Walaupun menggunakan ketepatan kaedah darjah kedua, ketepatan kadar konvergen kaedah NBF-VOF berpdudukan saiz grid merosot dari pada 2.0 kepada 1.5, perbandingan yang hampir dengan ujiikai diperoleh dari segi kulitifatif dan kuantitatif. The grid uncertainty obtained was less than 5%, which was within the ac-
ceptable range. Ketidakpastian grid diperoleh < 5%, berada pada anggaran yang boleh diterima. Masa pengiraan adalah rendah apabila menggunakan kelikatan pepejal yang tinggi. Tetapi kelikatan pepejal yang tinggi memberikan hasil yang ketinggalan untuk kes bergantung masa. Nisbah kelikatan antara pepejal dan cecair pada magnitud 100, memberikan keadaan optimum untuk kestabilan dan masa pengaliran. WAAlaubagaimanapun, menggunakan nombor Courant setinggi Co = 4, dapat mempercepatkan masa simulasi. Akhirnya, aplikasi kaedah ini telah dijalankan untuk mensimulasikan aliran darah MHV yang diletakkan dalam aorta simetri dan anatomik, yang mendedahkan corak aliran darah yang kompleks, beban tekanan ricih, dan tempoh masa sejarah zarah di domain setem-pat, yang seterusnya dapat mengenal pasti potensi pembekuan darah.
ACKNOWLEDGEMENTS

My deepest gratitude to my wife, Haslina Abdullah for her love and unwavering support throughout my entire graduate education, particularly toward the end. Her presence was the source of strength and inspiration for me to complete this thesis in which I will be eternally grateful. I am also thankful to my sons Faris, Firas, Faiq for their tears and laughter, which provided me a soothing comfort after those long hard days at work.

I owe a huge amount of gratitude to my committee members, especially to Associate Professor Dr. Ir. Kamarul Arifin Ahmad for sharing with me his knowledge, craftsmanship and wisdom in conducting scientific research. It has been a privilege to be his student. Special thanks to Associate Professor Dr. Farzad for being co-supervisor, and mentor for CFD. In addition, he also showed me the essentials of effective oral and written scientific presentations. To my other committee member, Professor Dr. Masaaki Tamagawa, whose providing Japanese style of guidance, Associate Professor Dr. Ahmad Fazli Abdul Aziz, for providing clinical discussion and medical data, and Associate Professor Dr. Surjatin Wiradirdja for his advise on managing research, and the continues supporting guidance. Many thanks also to all my friends and colleagues, such as Dr. Zuber, Adi Azriff, Vizy Nazira, Syed Aftab, Mohd Firdaus, and Ernzie Illyani, for their support and lively conversations. I am unable to mention all other names because the list will simply be too long.

Particular thanks to Universiti Putra Malaysia providing the High performance Computing (HPC) facilities. Finally, great appreciation must be extended to the Universiti Teknikal Malaysia Melaka, and Ministry of Higher Education Malaysia for providing the financial means for my graduate education. Without their generous support, this thesis would have never been written.
I certify that a Thesis Examination Committee has met on 25 April 2018 to conduct the final examination of Mohamad Shukri bin Zakaria on his thesis entitled "Development of Non-Boundary-Fitted Cartesian Grid Method for Numerical Simulation of Mechanical Heart Valve and the Potential for Blood Clotting" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Doctor of Philosophy.

Members of the Thesis Examination Committee were as follows:

**Faizal bin Mustapha, PhD**
Professor Ir.
Faculty of Engineering
Universiti Putra Malaysia
(Chairman)

**Mohd Khairul Anuar bin Mohd Ariffin, PhD**
Professor Ir.
Faculty of Engineering
Universiti Putra Malaysia
(Internal Examiner)

**Azmin Shakhirine bin Mohd Rafie, PhD**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Internal Examiner)

**Raghuvir Pai, PhD**
Professor
Manipal University
India
(External Examiner)

\[Signature\]

**NOR AINI AB. SHUKOR, PhD**
Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 28 June 2018
This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The members of the Supervisory Committee were as follows:

**Kamarul Arifin bin Ahmad, PhD**
Associate Professor, Ir.
Faculty of Engineering
Universiti Putra Malaysia
(Chairman)

**Surjatin Wiriadidjaja, PhD**
Associate Professor
Faculty of Engineering
Universiti Putra Malaysia
(Member)

**Ahmad Fazli Abdul Aziz, PhD**
Associate Professor
Faculty of Medicine and Health Sciences
Universiti Putra Malaysia
(Member)

**Farzad Ismail, PhD**
Associate Professor
School of Aerospace Engineering
Universiti Sains Malaysia
(Member)

**Masaaki Tamagawa, PhD**
Professor
Kyushu Institute of Technology
Japan
(Member)

**ROBIAH BINTI YUNUS, PhD**
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

vii
Declaration by graduate student

I hereby confirm that:

- this thesis is my original work;
- quotations, illustrations and citations have been duly referenced;
- this thesis has not been submitted previously or concurrently for any other degree at any other institutions;
- intellectual property from the thesis and copyright of thesis are fully-owned by Universiti Putra Malaysia, as according to the Universiti Putra Malaysia (Research) Rules 2012;
- written permission must be obtained from supervisor and the office of Deputy Vice-Chancellor (Research and Innovation) before thesis is published (in the form of written, printed or in electronic form) including books, journals, modules, proceedings, popular writings, seminar papers, manuscripts, posters, reports, lecture notes, learning modules or any other materials as stated in the Universiti Putra Malaysia (Research) Rules 2012;
- there is no plagiarism or data falsification/fabrication in the thesis, and scholarly integrity is upheld as according to the Universiti Putra Malaysia (Graduate Studies) Rules 2003 (Revision 2012-2013) and the Universiti Putra Malaysia (Research) Rules 2012. The thesis has undergone plagiarism detection software.

Signature: __________________________ Date: __________________________

Name and Matric No: Mohamad Shukri bin Zakaria (GS41335)
Declaration by Members of Supervisory Committee

This is to confirm that:
- the research conducted and the writing of this thesis was under our supervision;
- supervision responsibilities as stated in the Universiti Putra Malaysia (Graduate Studies) Rules 2003 (Revision 2012-2013) are adhered to.

Signature:
Name of Chairman of Supervisory Committee:  
Associate Professor Ir. Dr. Kamarul Arifin bin Ahmad

Signature:
Name of Member of Supervisory Committee:  
Associate Professor Dr. Surjatin Wirjadidjaja

Signature:
Name of Member of Supervisory Committee:  
Associate Professor Dr. Ahmad Fazli Abdul Aziz

Signature:
Name of Member of Supervisory Committee:  
Associate Professor Dr. Farzad bin Ismail

Signature:
Name of Chairman of Supervisory Committee:  
Professor Dr. Masaaki Tamagawa
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ABSTRACT</strong></td>
<td>i</td>
</tr>
<tr>
<td><strong>ABSTRAK</strong></td>
<td>iii</td>
</tr>
<tr>
<td><strong>ACKNOWLEDGEMENTS</strong></td>
<td>v</td>
</tr>
<tr>
<td><strong>APPROVAL</strong></td>
<td>vi</td>
</tr>
<tr>
<td><strong>LIST OF TABLES</strong></td>
<td>xiii</td>
</tr>
<tr>
<td><strong>LIST OF FIGURES</strong></td>
<td>xiv</td>
</tr>
<tr>
<td><strong>LIST OF ABBREVIATIONS</strong></td>
<td>xx</td>
</tr>
</tbody>
</table>

## CHAPTER 1
**INTRODUCTION**
1.1 Motivation 1
1.2 Computational Modelling of Cardiovascular Flow 3
1.3 Problem Statement 5
1.4 Research Objectives 6
1.5 Scopes of the Studies 7
1.6 Thesis Outline 8

## CHAPTER 2
**LITERATURE REVIEW**
2.1 Overview 9
2.2 Fluid Dynamics of Mechanical Heart Valve (MHV) on Blood Clotting 11
2.2.1 Role of Local Flow in Blood Clotting 14
2.2.2 Method for Estimating Blood Clotting 17
2.3 Numerical Methods 19
2.3.1 Boundary Fitted Method 19
2.3.2 Non-Boundary-Fitted Methods 20
2.3.3 Mathematical Model for Non-Boundary-Fitted Methods 28
2.4 Discretization of a General Scalar Transport Equation 31
2.4.1 Discretisation of Spatial Terms 32
2.4.2 Temporal Discretization 35
2.5 Turbulence Model 35
2.5.1 Turbulence Modelling in Mechanical Heart Valve 37
2.6 FSI on Blood Clot Estimation 40
2.7 Experimental Fluid Dynamics (EFD) for validation 41
2.8 Parametric MHV Study 43
2.8.1 Effects of Anatomical Model 43
2.8.2 Effects of Leaflet Dynamics 45
2.8.3 Effects of Valve Orientation 49
2.9 Issues and Current Research Directions 51
3 MATHEMATICAL MODELS AND NUMERICAL METHODS

3.1 Overview

3.2 New NBF-VOF Cartesian Grid Method
   3.2.1 Treatment I: Setting up high solid viscosity ($\mu_s \rightarrow \infty$)
   3.2.2 Treatment II: Introducing Artificial Term to the Systems of Linear Algebraic Equations
   3.2.3 Stability
   3.2.4 Numerical Experiment of New Developed Method

3.3 Choices of Numerical Scheme

3.4 Role of Compressive Term

3.5 Numerical Algorithm Step

3.6 Image-to-Computation Framework

3.7 Implementing and Numerical Setup in OpenFOAM

3.8 Validation and Verification

3.9 Solver Verification
   3.9.1 Hagen-Poiseuille Flow
   3.9.2 Lid-Driven Cavity with Embedded Solid

3.10 Solver Validation
   3.10.1 Lid-driven cavity
   3.10.2 Flow Over a Cylinder in a Free Stream
   3.10.3 Flow Over a Cylinder Asymmetrically Placed in a Channel
   3.10.4 Flow on a 90° Tube Bend

3.11 Patient Specific Aorta Flow

3.12 Summary

4 NUMERICAL SIMULATION OF MECHANICAL HEART VALVE

4.1 Overview

4.2 Computational Setup
   4.2.1 MHV Placed in Axisymmetric Aorta
   4.2.2 MHV Placed in Anatomic Aorta

4.3 Results and Discussions
   4.3.1 Validation on Steady Flow: Quantitative Comparison
   4.3.2 Validation on Pulsatile Flow: Qualitative Comparison
   4.3.3 Flow Analysis and Aerodynamic Characteristics on Blood Clot Potential

4.4 Summary

5 CONCLUSIONS AND RECOMMENDATIONS

5.1 Overview

5.2 Conclusions

5.3 Present Contributions

5.4 Limitation

5.5 Recommendation
5.5.1 Future Work on Numerical Development 155
5.5.2 Future Work on MHV Simulation 155

REFERENCES 157
APPENDICES 180
BIODATA OF STUDENT 186
LIST OF PUBLICATIONS 187
## LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1 Previous review of articles complemented by the present study</td>
<td>10</td>
</tr>
<tr>
<td>2.2 Type of MHVs and their blood clot influences</td>
<td>12</td>
</tr>
<tr>
<td>2.3 Blood clot factors</td>
<td>16</td>
</tr>
<tr>
<td>2.4 Estimation of blood clotting model</td>
<td>18</td>
</tr>
<tr>
<td>2.5 Comparison of different numerical methods for MHV simulation applications</td>
<td>26</td>
</tr>
<tr>
<td>2.6 Modification of forcing function for pseudo rigid solid treatment</td>
<td>29</td>
</tr>
<tr>
<td>2.7 Various recent turbulent model uses for MHV and the observation</td>
<td>38</td>
</tr>
<tr>
<td>2.8 Fixed leaflet MHV simulation</td>
<td>47</td>
</tr>
<tr>
<td>2.9 Summary of previous MHV numerical studies</td>
<td>54</td>
</tr>
<tr>
<td>3.1 Coordinate and corresponding $\alpha$ after initialization at interface region $0 &lt; \alpha &lt; 1$</td>
<td>72</td>
</tr>
<tr>
<td>3.2 $C_{\text{max}}$, $C_{\alpha}$, $\alpha_{\text{max}}$, $\alpha_{\text{min}}$, and $\Delta t$ over time</td>
<td>74</td>
</tr>
<tr>
<td>3.3 Summary of numerical setup used in present works</td>
<td>84</td>
</tr>
<tr>
<td>3.4 Numerical tests and its objective</td>
<td>88</td>
</tr>
<tr>
<td>3.5 Centreline velocity and $L_2$ error for various grid size $h$ and viscosity ratio $\frac{H_s}{\mu_f}$ of Poiseuille flow</td>
<td>92</td>
</tr>
<tr>
<td>3.6 $L_2$ Errors and convergence rates</td>
<td>96</td>
</tr>
<tr>
<td>3.7 Numerical error uncertainty analysis based on GCI approach. Variable is at $y/L = 0.24$</td>
<td>96</td>
</tr>
<tr>
<td>3.8 Lid-driven flow inside a 2D cavity showing location of the eddies. PE: primary eddy; BR: bottom right; BL: bottom left</td>
<td>99</td>
</tr>
<tr>
<td>3.9 Grid refinement study for the flow around cylinder with $Re = 40$</td>
<td>101</td>
</tr>
<tr>
<td>3.10 Physical parameters of the flow pattern around a circular cylinder at $Re = 40$: Recirculation length $L_w/d$, separation angle $\theta_s$, location of recirculation centre ($a/d, b/d$), and Strouhal number $St$</td>
<td>102</td>
</tr>
<tr>
<td>3.11 Comparison of $L_w$ and $\Delta P$ between present NBF-VOF Cartesian grid method and that of Schafer and Turek (1996)</td>
<td>106</td>
</tr>
<tr>
<td>3.12 Maximum velocity comparison with different grid resolutions</td>
<td>111</td>
</tr>
<tr>
<td>4.1 Grid setup for axisymmetric aorta model</td>
<td>126</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Similar pattern between postulated (da Vinci’s) and measured blood vortices in the aortic root (Source: Bissell et al., 2014)</td>
</tr>
<tr>
<td>1.2</td>
<td>Direction of blood through the valves</td>
</tr>
<tr>
<td>1.3</td>
<td>Schematic view comparison of grid structure between (a) BF, (b) NBF and (c) VOF methods</td>
</tr>
<tr>
<td>2.1</td>
<td>Types of mechanical heart valves: (a) Starr-Edwards caged ball valve; (b) Bjork Shiley tilting disc valve; (c) Medtronic Hall tilting disc valve; and (d) St Jude Medical Regent bileaflet valve (Source: Dangas, 2016)</td>
</tr>
<tr>
<td>2.2</td>
<td>Typical boundary condition for one cycle pulsatile flow showing opening phase (A-B), acceleration phase (B-C), peak flow phase (C-D), deceleration phase (D-E), and closing phase (E-A). Continuous line: Mass flow rate; dash line: Angle of the leaflet</td>
</tr>
<tr>
<td>2.3</td>
<td>(a) Clean MHV; (b) Explanted MHV showing complete immobilization of both leaflets due to blood clot (aortic view); (c) The same explanted MHV (ventricular view) (Source: Tirilomis, 2012)</td>
</tr>
<tr>
<td>2.4</td>
<td>Velocity field of a misaligned valve showing the flow separation, recirculation, and shed vortices (Source: Bluestein et al., 2002)</td>
</tr>
<tr>
<td>2.5</td>
<td>Definitions of IB nodes, where the velocities are reconstructed. Filled squares: IB nodes of the fluid with at least one shared solid cell; filled triangles: IB nodes of solid with at least one shared fluid cell (Source: Sotiropoulos and Yang, 2014a)</td>
</tr>
<tr>
<td>2.6</td>
<td>Sketch of the velocity interpolation procedure (Source: Fadlun et al., 2000)</td>
</tr>
<tr>
<td>2.7</td>
<td>Span-wise vorticity on central plane of MHV on pulsatile flow (Source: Yang, 2016)</td>
</tr>
<tr>
<td>2.8</td>
<td>Example of computational grids for the simulation of the flow around a valve placed within a S-shaped duct using (a) IB with cartesian grid, and (b) IB with with a curvilinear grid, so-called CURVIB method (Source: Roman et. al, 2009)</td>
</tr>
<tr>
<td>2.9</td>
<td>Definition of the domain that contains a surface of discontinuity Γ, fluid domain $\Omega_f$, and solid domain $\Omega_s$, in uniform Cartesian grid</td>
</tr>
<tr>
<td>2.10</td>
<td>Schematic shape of the discretized domain (the owner (P) and the neighbour (N) cells)</td>
</tr>
<tr>
<td>2.11</td>
<td>Comparison of 2D vorticity contour at Re = 5000 using different RANS models: (a) SA; (b) $k-\varepsilon$ (Source: Nguyen et al., 2012)</td>
</tr>
<tr>
<td>2.12</td>
<td>Comparison of velocity profiles for $k-\varepsilon$, SA, and LES turbulent model (Source: Kuan et al., 2014)</td>
</tr>
<tr>
<td>2.13</td>
<td>Vorticity structure appearance of two different turbulent models: (a) RANS; (b) hybrid RANS/LES (Source: Ge et al., 2005)</td>
</tr>
<tr>
<td>2.14</td>
<td>Comparison of measured instantaneous out-of-plane vorticity distribution with CFD simulation (Source: Dasi et al., 2007a,Yun et al., 2014)</td>
</tr>
</tbody>
</table>
2.15 Comparison of velocity profile between experimental measurements of (Ge et al., 2005) and several numerical simulations on MHV for (a) \( Re = 6000 \), and (b) \( Re = 750 \) at the cross-sectional location at \( X_c \)

2.16 Streamlines in the fully-opened phase (Source: Bang et al., 2006)

2.17 Computational domain of blood through (a) anatomically realistic aorta (Borazjani et al., 2008), (b) axisymmetric model (Borazjani et al., 2010), and (c) anatomically realistic aorta with LV (Source: Le and Sotiropoulos, 2012)

2.18 Comparison of flow field between fixed valve (for steady inflow \( Re = 800 \) and 4200) and pulsatile inflow) and moving valve. (a) The shear stress variation at the leading edge of the valve; (b) The transvalvular pressure drop variation (Source: Rosenfeld et al., 2002)

2.19 MHV orientations recommended by previous studies relative to the geometry of the aortic root (indicated by lines of valve symmetry through its central orifice), showing left coronary (LC) and right coronary (RC) (Source: Haya, 2015)

3.1 Methodology flowchart for NBF-VOF development and their implementation used in present study

3.2 Definition of interface boundary with the NBF-VOF Cartesian grid method for (a) \( 10 \times 10 \) grid, and (b) \( 20 \times 20 \) grid

3.3 Lid-driven cavity problem setup for algorithm stability test

3.4 The corresponding value of colour function \( \alpha \) at cell center at collocated grid. Dash line: exact location of solid-fluid boundary. Empty circle : \( \alpha = 0 \), filled circle: \( \alpha = 1 \)

3.5 Comparison of colour function \( \alpha \) and streamline between original (left panel) and modified \( H(u) \) (right panel) showing different time instant

3.6 Comparison of velocity profile between original and modified \( H(u) \) at \( y = 0.3 \) showing time instant (a) 1 s, (b) 5 s, (c) 8 s, and (d) 10 s. Interface of \( \alpha = 0.5 \) is at \( x = 0.5 \)

3.7 Comparison of velocity profile between original and modified \( H(u) \) at \( y = 0.4 \) showing time instant (a) 1 s, (b) 5 s, (c) 8 s, and (d) 10 s. Interface of \( \alpha = 0.5 \) is at \( x = 0.4 \) and 0.6

3.8 Comparison of velocity profile between original and modified \( H(u) \) at \( y = 0.5 \) showing time instant (a) 1 s, (b) 5 s, (c) 8 s, and (d) 10 s. Interface of \( \alpha = 0.5 \) is at \( x = 0.3 \) and 0.7

3.9 Spurious oscillation effect due to forcing function shows velocity magnitude versus time at xy coordinate \((0.3,0.5)\)

3.10 Setup for lid-driven cavity with embedded domain for differencing test case

3.11 Grid used in lid-driven cavity test, with \( 40 \times 40 \) for uniform grid

3.12 Lid-driven cavity case showing (a) streamline for LUD scheme, and (b) comparison of velocity profile for various schemes at line \( y = 0.5 \)

3.13 Comparison velocity profile for lid-driven cavity test between unstructured, structured grid and with that of Ghia et al. (1982) at line \( y = 0.5 \)
3.14 Transport of $\alpha$ in lid-driven cavity flow for (a) without interface compression term ($C_a = 0$), and (b) with interface compression term ($C_a = 1$). The initial position of the cylinder is on the black line. The visualized entity is shown for all values of $\alpha$ between 0.01 and 0.99.

3.15 Overview of the image-to-computation framework process: (a) Threshold and segmentation image data. Only the interested region is extracted (in this case, the aorta); (b) retained desired domain and map into CFD platform; (c) generate uniform background mesh that covered the selected computational domain.

3.16 Implementation of OpenFOAM working directory into NBF-VOF method.

3.17 Configuration of two-dimensional Poiseuille flow. The mesh shown is a coarser grid size of $a/5$ for clear visibility.

3.18 Poiseuille flow showing (a) comparison of velocity profile between NBF-VOF Cartesian grid method and the theoretical solution (Equation (3.39)), and (b) numerical $L_2$ error versus the grid distance on different $\mu_s/\mu_f$ constraints.

3.19 Transient Poiseuille flow using BF and NBF-VOF Cartesian grid methods on different $\mu_s/\mu_f$ constraints.

3.20 Comparison of computational time between the develop NBF-VOF Cartesian grid method and conventional BF grid methods on Poiseuille flow.

3.21 Analysis of time step and $Co$ number for transient Poiseuille flow.

3.22 Lid-driven cavity with embedded solid showing (a) colour function contour on uniform mesh $60 \times 60$ (grid size $L/50$), and (b) the resulting velocity streamline.

3.23 Lid-driven cavity with embedded solid problem showing numerical $L_2$ error versus the grid distance in logarithmic scale for viscosity ratios $10^3$ and $10^6$.

3.24 Geometrical layout of the flow domain. $\alpha = 0$ is fluid domain, and $\alpha = 1$ is solid domain.

3.25 Comparison of velocity profile for lid-driven cavity flow at centreline of the cavity between developed NBF-VOF Cartesian grid method and with that of Ghia et al. (1982) showing (a) $u_x$ velocity profile along $x = 0.5$, and (b) $u_y$ velocity profile along $y = 0.5$.

3.26 Comparison of streamline pattern for the 2D lid-driven cavity flow at $Re = 1000$ between (a) the developed NBF-VOF Cartesian grid solution, (b) the work of Ghia et al. (1982).

3.27 Schematic view of the flow over a cylinder in a free stream with dimension.

3.28 Zoom view of the NBF-VOF Cartesian grid method on coarse grid at vicinity of cylinder.

3.29 Time evolution of the recirculation length with three grid sizes.

3.30 Flow past a circular cylinder showing (a) streamline visualization for $Re = 20$, (b) streamline visualization for $Re = 40$, and (c) parameter definition.
3.31 Flow past a circular cylinder at $Re = 40$ showing a comparison of pressure coefficient $C_p$ between NBF-VOF, BF grid method (Tseng and Ferziger, 2003), and experimental measurements (Grove et al., 1964)

3.32 Flow around a cylinder for $Re = 100$ showing (a) the vorticity field, and (b) the vertical velocity versus time for $St$ estimation. The $u_y$ was measured at probe A

3.33 Geometry setup with boundary conditions for flow over a cylinder asymmetrically places in a channel

3.34 Flow over a cylinder asymmetrically places in a channel showing streamline visualization for (a) $Re = 20$, and (b) $Re = 100$

3.35 Geometry setup for a 90° bend tube flow. The coarse size of NBF grid is shown ($\Delta x = \Delta y = d/8$)

3.36 Numerical-experimental comparison of stream wise velocity versus normalise tube diameter 90° tube bend for (a) $\theta = 0^\circ$, (b) $\theta = 23.4^\circ$, (c) $\theta = 58.5^\circ$, and (d) $\theta = 81.9^\circ$, respectively. Normalise distance = 1 for inner curve, and normalise distance = 0 for outer curve

3.37 Velocity contour maps: (a) $0^\circ$, (b) $22.5^\circ$, (c) $45^\circ$, (d) $67.5^\circ$ and (e) $90^\circ$, (I: inner curve, O: outer curve). The results presented in the upper half of the figure were derived by De Vosse et al. (1989). Present numerical results are provided in the bottom half

3.38 Mesh structure for the (a) BF and (b) NBF-VOF Cartesian grid methods

3.39 Grid independency test of velocity profile using at cross-section location $y = -0.188$ for (a) NBF-VOF Cartesian grid and (b) BF grid methods. The corresponding coordinate is shown for (c) NBF-VOF Cartesian grid method, and (d) BF grid method

3.40 Velocity contour comparison between the BF and NBF grid methods at eleven cross-section locations during the peak flow instant time. The left bottom subfigure the pulsatile flow impose at the inlet

3.41 Velocity contour of $u_z$ at Cross-section B using the (a) NBF-uniform mesh and (b) BF (conventional), (I: inner curve, O: outer curve)

3.42 Velocity profile ($u_z$) at Cross-section B along the line (a) $y = -0.18$; (b) $y = -0.188$, (c) $y = -0.194$, and (d) $y = -0.2$. Refer to Figure 3.39c & d for the respective cross-section location

3.43 Comparison of velocity streamline between the BF (a) and NBF-VOF Cartesian grid method (b) shows the helical flow profile in the aorta curvature during the peak flow

3.44 Instantaneous vortical structure by the Q-criterion ($Q = 5000$), coloured by velocity magnitude, obtained using newly developed NBF-VOF Cartesian grid and conventional BF grid methods at different instantaneous pulsation time

4.1 MHV in axisymmetric aorta flow direction showing the colour function $\alpha$

4.2 MHV in anatomy aorta flow direction showing the colour function $\alpha$

4.3 The flow methodology for MHV simulation analysis. Yellow-filled: Axisymmetric aorta model; blue-filled: Anatomic aorta model
4.4 Pulsatile inflow used in present study for MHV simulation. The analysis concentrate on three instant time namely, accelerating flow (AF) \( (t = 0.25 \text{ s}) \), peak flow (PF) \( (t = 0.45 \text{ s}) \) and decelerating flow (DF) \( (t = 0.45 \text{ s}) \).

4.5 Axisymmetric, straight test section. Geometry similar to that used by Dasi et al. (2007).

4.6 Numerical geometry of the MHV in axisymmetric aortic root model showing the grid topology.

4.7 Grid dependency test for axisymmetric aorta at \( Re = 750, x = 32 \text{ mm} \). See Figure 4.1 for the plotted line reference.

4.8 Segmentated images aorta from CT scan.

4.9 Combination of tube and anatomic sinus.

4.10 Numerical geometry of the MHV in anatomy aorta showing the grid topology.

4.11 Grid dependency test for anatomic aorta at \( Re = 750, x = 45 \text{ mm} \). See Figure 4.2 for the plotted line reference.

4.12 Experimental-numerical comparison for steady flow at \( Re = 750 \), for (a) near leaflet tips \( (x = 32 \text{ mm}) \), (b) middle of sinus \( (x = 48 \text{ mm}) \), and (c) end of sinus \( (x = 61 \text{ mm}) \). See Figure 4.1 for the plotted line reference.

4.13 Experimental-numerical comparison for steady flow at \( Re = 6000 \), for (a) near leaflet tips \( (x = 32 \text{ mm}) \), (b) middle of sinus \( (x = 48 \text{ mm}) \), and (c) end of sinus \( (x = 61 \text{ mm}) \). See Figure 4.1 for the plotted line reference.

4.14 Comparison of 2D vorticity between present NBF-VOF Cartesian grid method, previous simulation (Yun et al., 2014b) and experiments measurement (Yun et al., 2014b) during PF phases.

4.15 Comparison of vorticity contour using different turbulence models: (a) SA (Nguyen et al., 2012); (b) \( k - \varepsilon \) (Nguyen et al., 2012); (c) URANS (Ge et al., 2005); (d) DES (Ge et al., 2005); and (e) LES, present NBF-VOF Cartesian grid method.

4.16 Velocity magnitude at the central \( xy \) plane for (a) anatomic, AF, (b) axisymmetric, AF, (c) anatomic, PF, (d) axisymmetric, PF, (e) Anatomic, DF, and (f) axisymmetric, DF.

4.17 Velocity vector at the central \( xy \) plane during PF for (a) axisymmetric aorta case and (b) anatomic aorta case.

4.18 Streamline pattern at the central \( xy \) plane during PF for (a) anatomic and (b) axisymmetric aorta. The point source of the streamline is taken at the tip of the leaflet with radius 0.005.

4.19 Streamline pattern for anatomic model during (a) AF (b) PF and (c) DF.

4.20 2D vorticity contour at the central \( xy \) plane for (a) anatomic, AF, (b) axisymmetric, AF, (c) anatomic, PF, (d) axisymmetric, PF, (e) anatomic, DF, and (f) axisymmetric, DF.

4.21 Instantaneous vortical structures visualised by iso-surfaces of \( \lambda_2a = -10000 \) for an anatomic aorta.

4.22 TKE contour at time instant PA for (a) anatomic, \( xy \) plane, (b) anatomic, \( xz \) plane, (c) axisymmetric, \( xy \) plane, and (d) axisymmetric, \( xz \) plane.
4.23 Viscous stress contour at the central $xy$ plane for (a) anatomic, AF, (b) axisymmetric, AF, (c) anatomic, PF; (d) axisymmetric, PF, (e) anatomic, DF; and (f) Axisymmetric, DF. With contour scaling capped at $\tau_{eq} = 10$ Pa.

4.24 Viscous stress contour at $xz$ plane during PF for (a) bottom leaflet (b) top leaflet, and (c) between leaflets

4.25 Viscous stress contour at $yz$ plane during PF at (a) trailing, (b) middle, and (c) leading edge of leaflet

4.26 Comparison of viscous stresses profile at vicinity area of leading edge of the leaflet for a complete cardiac cycle

4.27 Comparison of viscous stresses profile at the central $xy$ plane for (a) anatomic, leaflet tip, $x = 45$ mm, (b) anatomic, sinus middle, $x = 55$ mm, (c) anatomic, end of sinus, $x = 63$ mm, (d) axisymmetric, leaflet tip at $x = 32$ mm, (e) axisymmetric, sinus middle, $x = 48$ mm, and (f) Axisymmetric, end of sinus, $x = 61$ mm

4.28 Seeded particle for corresponding flow time showing particle age in seconds

B.1 Anatomic geometry of aorta with valve showing (a) front view (y plane) (b) top view (z plane) and (c) side view (x plane)

B.2 Modeled geometry of aorta with valve showing (a) side view, (b) front view, and (c) top view
LIST OF ABBREVIATIONS

AF accelerating flow
ALE arbitrary lagrangian eulerian
ATS american thoracic society
avg average
BD blended differencing
BDI blood damage indexes
BF boundary fitted
BHV bioprosthetic heart valve
BMHV bileaflet mechanical heart valve
CD central differencing
CFD computational fluid dynamics
CPU central processing unit
CT computed tomography
CURVIB curvilinear immersed boundary method
CVD cardiovascular diseases
DES detached eddy simulation
DF decelerating flow
DFG Deutsche Forschungsgemeinschaft (German Research Association)
DNS direct numerical simulation
EFD experimental fluid dynamics
FCT flux corrected transport
FD fictitious domain
Fs safety factor
FVM finite volume method
GCI grid convergence index
IB immersed boundary
IIM immersed interface method
IJN Institut Jantung Negara (National Health Institute)
IMM immersed membrane method
LBM lattice boltzman method
LC left coronary
LES large eddy simulation
LUD Linear upwind differencing
LV left ventricle
MHV mechanical heart valve
MPI message passing interface
MRI magnetic resonance imaging
MULES Multi-dimensionsal limiter for explicit solution
NBF non-boundary fitted
NBF-VOF non-boundary fitted/volume of fluid
PCG preconditioned conjugate gradient
PDEs partial differential equations
PF
PIV
PLIC
RANS
RBC
RC
RSS
SA
SGS
sim
SJM
SLIC
SPH
SST
TSS
TVD
URANS
UD
VS
VOF
w
WSS
XFEM

Symbol

\( a \)
\( a, b \)
\( [A] \)
\( C \)
\( C_{\alpha} \)
\( C_k, C_e \)
\( C_p \)
\( C_u \)
\( d \)
\( f \)
\( F \)
\( f_N \)
\( G \)
\( h \)
\( H \)
\( H(U) \)
\( H(U)^* \)
\( I_{red} \)
\( K \)
\( k_{SGS} \)
\( L_w \)

peak flow
particle image velocimetry
piecewise linear interface construction
reynolds average navier stokes
red blood cell
right coronary
reynolds shear stress
spalart almaras
sub-grid scale
simulation
st jude medical
simple line interface calculation
smooth particle hydrodynamics
shear stress transport
turbulent shear stress
total variation diminishing
unsteady reynolds average navier stokes
upwind differencing
vortical structural
volume of fluid
width
wall shear stress
extended finite element method

matrix coefficient
recirculation length location for the flow around cylinder
squared matrix of the coefficients
model constants for BDI
courant number
interface courant number
turbulent coefficient for LES
pressure coefficient
turbulent variable dependent on the rate of deformation and spin tensors
diameter
forcing function
flux
distance between center of cell P and face center of cell P
elasticity coefficient
grid size
height
original off-diagonal matrices coefficient
modified off-diagonal matrices coefficient
reduced moment of inertia
dean number
turbulent kinetic energy
recirculation length
\( L_2 \)  
error norm

\( \mathbf{n} \)  
normal direction

\( \mathbf{n}_f \)  
normal vector of the cell surface

\( N \)  
total number of grid

\( P \)  
pressure

\( p \)  
order of accuracy

\( P_{\infty} \)  
free stream Pressure

\( P\overline{N} \)  
distance between center of cell P and center of cell N

\( Q \)  
second tensor invariant

\( [R] \)  
source term vector

\( r \)  
smoothness monitor or r-factor for TVD differencing schemes 
or grid refinement ratio

\( Re \)  
reynolds number

\( R_c \)  
radius of curvature for bend

\( S \)  
deformation rate (strain-rate) tensor or surface area vector 
or symmetric part of the velocity gradient

\( S_{tl} \)  
strouhal number

\( S_p \)  
linear part of the source term

\( S_{u} \)  
constant part of the source term

\( S_0 \)  
source term

\( t \)  
time

\( \mathbf{u} \)  
velocity vector

\( u \)  
velocity magnitude

\( \mathbf{u}_c \)  
relative velocity

\( V \)  
volume

\( \omega \)  
vorticity

\((x_a,y_a)\)  
coordinate at front of cylinder

\((x_e,y_e)\)  
coordinate at end of cylinder

**Greek**

\( \alpha \)  
VOF color function

\( \alpha_{max} \)  
maximum value of color function

\( \alpha_{min} \)  
minimum value of color function

\( \Gamma \)  
interface or diffusivity

\( \gamma \)  
forcing function constant

\( \delta \)  
curvature ratio of the tube bend

\( \Delta \)  
difference

\( \Delta t \)  
time step size

\( \Delta t_{max} \)  
max time step

\( \epsilon \)  
turbulent energy dissipation, Penalization parameter

\( \zeta \)  
damping coefficient

\( \eta \)  
forcing function constant

\( \theta \)  
angle or leaflet’s angle

\( \theta_s \)  
separation angle

\( \kappa \)  
interface curvature or bulk viscosity

\( \lambda \)  
lagrange multiplier or tensor eigenvalue

\( \lambda_2 \)  
second invariant of tensor

\( \lambda_1, \lambda_2 \)  
adaptive time step coefficient
\mu \quad \text{dynamic viscosity}
\mu_f \quad \text{fluid dynamic viscosity}
\mu_s \quad \text{solid dynamic viscosity}
\mu_t \quad \text{turbulent dynamic viscosity}
\mu_{SGS} \quad \text{eddy viscosity}
\nu \quad \text{kinematic viscosity}
\rho \quad \text{density}
\sigma \quad \text{surface tension}
\tau \quad \text{shear stress or period of vortex shedding}
\tau_w \quad \text{wall shear stress}
\tau_{eq} \quad \text{equivalent shear stress}
\tau_e \quad \text{stress tensor for hyperelastic material}
\phi \quad \text{general scalar property}
\xi \quad \text{moment around the hinge axis}
\Omega \quad \text{antisymmetric parts of the velocity gradient}
\Omega_f \quad \text{Continuous of fluid domain}
\Omega_s \quad \text{embedded or solid domain}
\psi \quad \text{TVD limiter}
\Omega_1 \quad \text{continuous domain properties}
\Omega_2 \quad \text{embedded domain properties}

\text{Superscripts}
', \tau \quad \text{transpose}
\alpha \quad \text{model constants for BDI}
\beta \quad \text{model constants for BDI}
n \quad \text{discrete time level}
L \quad \text{linear term for the flux F}
NL \quad \text{non-linear term for the flux F}
\phi \quad \text{filtered variable}

\text{Subscripts}
(i,j) \quad \text{(x,y) cell coordinates}
x, y, z \quad \text{coordinate components}
f \quad \text{face interpolation}
N \quad \text{neighbouring cell N}
P \quad \text{owner cell P}
SGS \quad \text{turbulent SGS properties}
CHAPTER 1

INTRODUCTION

1.1 Motivation

Imagine that a person has accidentally cut his finger. After some time, the blood will begin to clot to stop the finger from bleeding. That is the good function of blood clotting. However, if a blood clot develops in a patient's heart valve due to some abnormal flow, there is a possibility that the clot may break off and go to the brain (causing a stroke) or to other organs in the body. In certain cases, the blood could clot at the valve itself and cause it to malfunction. To avoid this, blood thinners (usually warfarin) must be taken at the right dosage everyday with periodic blood tests and dietary restrictions (Cannegieter et al., 1994; Shoeb and Fang, 2013). This routine may change the lifestyle of the patient. A second complication is bleeding due to the use of blood thinners. A patient taking a blood thinner may encounter a problem when he is injured or requires surgery, whereby during the surgery, the use of the blood thinner has to be controlled to prevent excessive bleeding during the operation. This puts the patient at risk. It has been reported that the risk of both bleeding and blood clots is 1-2% each year. Therefore, for a patient who receives an artificial heart valve at the age of 40 years and lives to the age of 80 years, there is a 40-80% chance of both bleeding and blood clotting occurring (Shoeb and Fang, 2013). Moreover, the use of blood thinners will also cause birth mortality among young women who wish to have children (Vitale et al., 1999; Neumann et al., 2016).

Scientific knowledge of the heart dates back as far as the beginnings of recorded history. Among the first people to investigate and write about the anatomy of the heart was the Greek physician, Erasistratus (around 250 BC), and Claudius Galenus (around 129-201) who was a Greek-born Roman physician. Later, Leonardo da Vinci (1452-1519) also made some advances in the understanding of blood flow (Gharib et al., 2002). Briefly, da Vinci believed that the valve was closed during a forward flow by the vortex that forms behind the valve leaflets through his drawing in Figure 1.1. Nevertheless, after nearly 500 years later, finding an accurate quantitative description of the cardiac function still poses a challenge. Only just recently, in 2014, da Vinci’s vortex formation and re-circulation were reported in-vivo (Bissell et al., 2014) and in-vitro (Querzoli et al., 2014) studies and direct comparison have been made.
Cardiovascular disease (CVD) remains the leading global cause of death, accounting for more than 17.3 million deaths per year in 2013 worldwide, according to the American Heart Association’s 2017 Heart Disease and Stroke Statistics Update (Benjamin et al., 2017). It represents 31% of all global deaths, a number that is expected to grow to more than 23.6 million by 2030. More than 75% of CVD deaths occur in low-income and middle-income countries, and 80% of all CVD deaths are due to heart attacks and strokes.

One of the CVD is associated with the malfunction of heart valves such as stenosis (heart valve that does not open properly) and regurgitation (backflow of blood as the valves are closing). Figure 1.2 shows the flow direction of blood through the valves. Unrepaired valves necessitate surgery so that the artificial heart valves replacement can be done. It is estimated that more than 300,000 replacement heart valves are implanted annually worldwide (Jahandardoost et al., 2016). Since the first implantation of artificial heart valves in 1952, significant risks, such as the need for anticoagulation drugs and re-surgery operation, are still present. Current artificial heart valves suffer from several problems such as blood cell damage (haemolysis) and formation of the blood clot (thrombosis) (Yoganathan et al., 2004; Borazjani, 2015; Bark et al., 2016). This complication requires patients to undergo anticoagulant therapy, which may lead to life-threatening haemorrhage or stroke if poorly managed.
1.2 Computational Modelling of Cardiovascular Flow

A thorough understanding of the aerodynamic characteristics in blood flow is needed to improved artificial heart valve performance. Although the measurement of aerodynamic properties through current advance medical imaging devices are feasible, such as magnetic resonance imaging (MRI), computed tomography (CT) scans, and echocardiography (Mittal et al., 2016), it remains to be a complicated process for determining the local influence of fluid mechanical factors such as viscous stress on the blood constituents (Yokoi et al., 2005). Furthermore, experimental work in this focus area is expensive and limited. Alternatively, using mathematical equations through a numerical method and simulation should be adopted.

Being able to look into the heart through mathematical equations would be a fantastic achievement. The visualisation of the blood flow behaviours in the heart, for example through the heart valve has become an interest in the computational fluid dynamics (CFD) community for the last few decades due to the increasing use of supercomputer nowadays.
CFD simulations can provide valuable information to the medical device manufacturers and surgeons in making critical decisions in the treatment of heart valve repair or replacements. The visualisation will enable them to access the level of disease (such as blood clotting) in great detail. Whether either CFD information will allow access to the level of disease in great detail or not, it will continue to be the subject of intense debate in literature (Yun et al., 2014a; Jahandardoost et al., 2016).

Nevertheless, CFD modelling is widely used to unravel many engineering problems, for example, in the design and manufacturing of aircrafts (Ahmad et al., 2005; Firdaus et al., 2016; Ismail and Roe, 2009; Aftab et al., 2016), marine technology (Carrica et al., 2013; Zakaria et al., 2013), electronic cooling (Abdullah et al., 2009), and recently in the biomedical field (Riazuddin et al., 2010; Zakaria et al., 2016; Basri et al., 2016). Many of these engineering problems involve complex geometries that do not fit exactly in Cartesian co-ordinates (Versteeg and Malalasekera, 2007). When the flow boundary does not coincide with the co-ordinate lines of a cartesian grid, one could proceed by non-Cartesian grid coordinate systems (i.e. cylindrical, axisymmetric three-dimensional or spherical co-ordinates). For the worst cases, randomized, skewed and distorted grid may be used.

Grid generation represents a critical step in modelling complex geometry and is usually performed using unstructured meshing algorithms conforming to the surface geometry which leads to poor mesh generation. The poor mesh in turn will influence the accuracy, stability and convergence of the numerical solution. Although hexahedral Cartesian meshes are known to provide a higher accuracy and reduce the computational costs, their application in computational cardiovascular studies is challenging due to the complex and branching topology of vascular territories. Due to this restraint, the use of accurate CFD simulations in the medical field is still sparse in literature, and its numerical development continues to be of major interest in research.

There are two main types of grid meshes for complex geometry; boundary fitted (BF) methods and non-boundary-fitted (NBF) methods. BF volume mesh is created around the imported geometry. The BF method will usually generate a poor unstructured tetrahedral mesh quality. Poor quality surface and volume meshes can result in difficulties with the solution of the flow problem, ranging from inaccurate solutions to non-convergence of the solution process. Therefore, to generate a high-quality mesh, significant user effort is usually required to perform the meshing procedure at the boundary when the boundary-fitted (BF) grid method is used. This task is an additional burden and is tedious. With the NBF method, the underlying grid does not coincide with the geometry of the surface being treated, thus efficiently generating the Cartesian hexahedral mesh.

The earlier study of fluid flow using the NBF method in the biomedical field was done by Peskin (1977), where the so-called immersed boundary (IB) method was introduced to simulate the fluid flow problem in a heart valve. Later, further improvements to the method were developed such as the fictitious domain method (Glowinski et al., 1999; Yu et al., 2013), cut cell method (Meinke et al., 2013; Qin and Krivodonova, 2013), and
ghost fluid method (Fedkiw et al., 1999; Liu, 2014), just to name a few. These methods use local forcing function to identify a solid object, which comes with several issues such as unaligned between boundary and grid, blur interface, and stiffness of the governing equations. Another method is volume of fluid (VOF) (Hirt and Nichols, 1981; Takagi et al., 2012) mostly used to solve multiphase fluid flow problem. In VOF method, colour function $\alpha$ is used to distinguish between fluid and solid, where $\alpha = 1$ is solid, and $\alpha = 0$ is fluid. The implementation VOF method for fluid-solid geometry is sparse but rarely can be found in literature such as in (Ravoux et al., 2003; Ng, 2009). A schematic view comparison between the traditional BF, common NBF and VOF methods representation grid is shown in Figure 1.3.

![Figure 1.3: Schematic view comparison of grid structure between (a) BF, (b) NBF and (c) VOF methods](image)

In this work, a robust procedure of new NBF method combining with VOF method without the local forcing function was proposed. The methodology adopted in this work is designed so that it could be suitably implemented in an open source code, OpenFOAM, and could be used to solve fluid flow problems in the biomedical field faced by scientists and researchers. Such a numerical study may not require substantial changes to existing CFD codes, particularly those codes done in-house by specific researchers. Furthermore, medical imaging techniques provide the multi-component geometry as voxel data for each patient, which would share the same ground as the Cartesian grid VOF colour function. As far as the authors know, present work is the first to implement an NBF grid technique through a simple extension of the VOF interface capturing scheme, particularly for MHV flow in blood clotting estimation.

### 1.3 Problem Statement

The MHV is prone to blood clotting. A blood clot can be estimated from the accumulation of the shear stress and residence time of the platelet. For the Newtonian fluid, the shear stress was proportional to the velocity gradient. The velocity gradient can yield the complex flow such as vorticity, stagnation flow, and separation. To be able to capture this rich dynamic complex flow structure in pulsation and highly turbulent flow, high order accurate numerical methods are needed to discretising and solving the governing equations numerically.
The numerical accuracy and stability are mainly influenced by the mesh quality. For a simple 2D test case on uniform Cartesian grids, a second-order method should remain close to the second-order accuracy. However, when the grids are uniformly distorted (skewed), a second-order finite volume method (FVM) can drop to less than the second-order (Ismail et al., 2010; Chizari and Ismail, 2015). Furthermore, in randomised grids, a second-order FVM can behave very erratically (negative order of accuracy) (Chizari and Ismail, 2016). The meshing for complex geometry using conventional BF method is always either unstructured, high aspect ratio, high skewness, or non-orthogonal. These characteristics affect the accuracy and stability of the numerical method. To ensure uniform Cartesian grid used for the whole computational domain regardless the complexity of the geometry, non-boundary-fitted (NBF) grid method is a perfect candidate.

However, previous NBF grid method faced several issues. Firstly, the grid point did not necessarily coincide with the boundary node (Fadlun et al., 2000); making interpolating the velocity is necessary. Secondly, the resolution at the interface is smeared in a few grid cells, thus required very fine mesh at the interface. Finally, the forcing function in previous NBF method required a user-defined parameter. This parameter must be chosen in such a way that to balance between producing solid nature of embedded domain and to avoid numerical oscillation, at a reasonable computational cost. Too large forcing function parameter will increase the stiffness of the governing equations and, therefore, affect convergence properties (Engels et al., 2015).

Therefore, this study intends to fill the gap of knowledge to develop a new NBF method for a pseudo-rigid-body, using the idea of mixture properties of viscosity \( \mu \) and colour function \( \alpha \) of the volume of fluid (VOF). As no additional forcing function is needed, the new method hypothesises that the global user defines parameters that do not affect the overall accuracy, convergence and total computational cost. The newly developed method will be demonstrated for the first time with real MHV flow implant in the aorta to see the potential of blood clotting. It is hypothesised that the developed method is feasible for modelling the blood flow in through MHV in the aorta.

1.4 Research Objectives

The ultimate goal of this research is to develop a new fluid flow numerical method using NBF grid method on the Cartesian grid for the flow on a complex stationary domain. The method must be able to integrate medical images and accurately simulate the flow field through the heart valves, showing the non-physiological flow patterns, responsible for blood clotting. To achieve this objective, the focus of the thesis will be on the following specific aims:

1. To identify issues and current research direction on numerical method, and aerody-
namics characteristics on blood clot potential for MHV simulation.

2. To develop a new Cartesian NBF grid method for complex geometry namely, non-boundary-fitted/volume of fluid (NBF-VOF) Cartesian grid method.

3. To validate a new develop NBF-VOF Cartesian grid method with conventional BF method, previous NBF method, and previous experimental result using a series of benchmark tests.

4. To verify the develop NBF-VOF Cartesian grid method in simulating blood flow through the MHV located in an axisymmetric and anatomic aorta to access the flow pattern and location of blood clot potential.

1.5 Scopes of the Studies

The present study was bounded by the following scopes,

1. This study involved numerical works, where a new mathematical method was introduced and integrated with OpenSource OpenFOAM CFD platform via editable C++ code. Nevertheless, to validate the solver, comparison with available numerical and experimental data was made. For MHV, existing experimental work in literature was used for validation purposes.

2. The turbulent model available in the literature varied, ranging from RANS, LES and DNS. In this study, only one model was used, which was the LES turbulent model, since a previous study (Nguyen et al., 2012) reported it could handle rich dynamic flow field in MHV. Furthermore, LES is more superior than common RANS model because it can solve instantaneous details of flow field, which is required in blood clot formation simulation (Anupindi et al., 2013; Yun et al., 2014b). Therefore, investigating or implementation of any other turbulent model is currently beyond the scope of the study.

3. Among the variety of MHV available in the market for clinical practice, present study used the St Jude Mechanical (SJM) heart valve model as the computational model. This type has good hemodynamic flow and covers over 80% implanted into the patient (Mirkhani et al., 2016). It has plenty of numerical and experimental data solution. Furthermore, many researchers use them as a model for CFD code validation purpose (i.e. (Yun et al., 2014b; Jahandardoost et al., 2016)).

4. The leaflet was treat stationary which is sufficient to access the blood clot potential. Therefore, present study developed a method that was suitable for fixed boundaries only, and the fixed valve’s leaflet was chosen instead.

5. The blood properties were assumed to be Newtonian since the size of the heart and surrounding blood vessels was larger by at least three orders of magnitude than
the typical blood cell (the typical size of blood cells is of the order of 10 µm). Therefore, when considering flow phenomena associated with heart valves, it is treated blood, for the most part, as a continuum medium that was incompressible and Newtonian (Sotiropoulos et al., 2016). Therefore discussion up to molecular level is also beyond the scope of the study.

1.6 Thesis Outline

This thesis is divided into five chapters including an introductory chapter (Chapter 1). Followed by Chapter 2, where present study provided the comprehensive literature review concerning numerical methodologies for the solution of the BF and NBF method, method for estimating blood clotting, experimental cases suitable for the heart valve validation, and some parametric study that contribute to blood clotting.

Furthermore, Chapter 3 is the primary framework of this thesis where the gap was illustrated. The mathematical formulation and solution strategy for the modified NBF method, namely NBF-VOF grid method is shown. This chapter also show the bridging between previous old method to present new method. Two treatments were made: 1) impose high viscous solid and 2) modification of the linear system of Navier-Stokes equations. In Chapter 3, a comprehensive validation and verification was also done. The validation data was taken from analytical solution, established existing numerical and experimental data. Furthermore, the new method also validated using conventional BF method with real aorta vessel as test geometry.

Moreover, Chapter 4 discusses the application or practical contribution of current NBF-VOF method in a real complex geometry of medical image data. Although the validation of the solver is extensively done in Chapter 3, present study continue to provide the model validation using asymmetric aorta case, where an experimental and numerical solution exists. Present study also compared the flow field between the axisymmetric and anatomic aorta and accessed the potential of blood clot potential.

Finally, the conclusion of the entire finding is done in Chapter 5 together with a recommendation for future work. It is also worth to mention that some content of this thesis has been published in journal articles and the list of publication is presented in the appropriate section.
REFERENCES


162


170


