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

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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

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

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April 2018

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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 descretisation 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^o 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

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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.

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Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

PEMBANGUNAN KAEDAH GRID-TIDAK-TERIKAT UNTUK SIMULASI BERANGKA PADA INJAP JANTUNG MEKANIKAL DAN POTENSI UNTUK PEMBEKUAN DARAH

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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 mekanik (MHV). Kajian terdahulu menunjukkan bahawa corak aliran bukan fisiologi, menyebabkan platelet terperangkap, bertanggungjawab ke atas pembentukan darah beku pada MHV. Ketepatan simulasi aliran ini memerlukan darjah ketepatan yang tinggi dengan skala yang dapat menyelesaikan masalah pergolakan seperti simulasi eddy besar (LES). Ini memerlukan penggunaan grid ortogonal seragam, yang tidak dapat dikendalikan oleh bentuk arteri yang komplek yang mengandungi 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 mengenali kedua-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 dapati bahawa, kaedah itu tidak memuaskan. Untuk terus menyekat halaju 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^o aliran tiub, dan aliran denyutan melalui aorta anatomik sebenar. Kesamaan yang sangat baik telah dihasilkan untuk semua kes. Walaupun menggunakan ketepatan kaedah darjah kedua, ketepatan kadar konvergen kaedah NBF-VOF berpndukan saiz grid merosot daripada 2.0 kepada 1.5, perbandingan yang hampir dengan ujikaji diperoleh dari segi kulitatif dan kuantitatif. The grid uncertainty obtained was less than 5%, which was within the ac-

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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. WAlaubagaimanapun, 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 setempat,yang seterusnya dapat mengenal pasti potensi pembekuan darah.

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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 Wiriadidjaja 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 Ernnie 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.

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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:

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LIST OF ABBREVIATIONS

AF	accelerating flow
ALE	arbitrary lagrangian eulerian
ATS	american thoracic society
avg	average
BD	blended bifferencing
BDI	blood damage indexs
BF	boundary fitted
BHV	bioprosthetic heart valve
BMHV	bileaflet mechanical heart valve
CD	central cifferencing
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

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PF	peak flow
PIV	particle image velocimetry
PLIC	piecewise linear interface construction
RANS	reynolds average navier stokes
RBC	red blood cell
RC	right coronary
RSS	reynolds shear stress
SA	spalart almaras
SGS	sub-grid scale
sim	simulation
SJM	st jude medical
SLIC	simple line interface calculation
SPH	smooth particle hydrodynamics
SST	shear stress transport
TSS	turbulent shear stress
TVD	total variation diminishing
URANS	unsteady reynolds average navier stokes
UD	upwind differencing
VS	vortical structural
VOF	volume of fluid
w	width
WSS	wall shear stress
XFEM	extended finite element method

Symbol

a	matrix coefficient
a, b	recirculation length location for the flow around cylinder
$[A]$	squared matrix of the coefficients
C	model constants for BDI
Co	courant number
Co_{α}	interface courant number
C_k, C_e	turbulent coefficient for LES
C_p	pressure coefficient
C_u	turbulent variable dependent on the rate of deformation and spin tensors
d	diameter
$\mathbf{f}$	forcing function
F	flux
$\overline{fN}$	distance between center of cell P and face center of cell P
G	elasticity coefficient
h	grid size
H	height
$\mathbf{H}(\mathbf{U})$	original off-diagonal matrices coefficient
$\mathbf{H}(\mathbf{U})^*$	modified off-diagonal matrices coefficient
I_{red}	reduced moment of inertia
K	dean number
k_{SGS}	turbulent kinetic energy
L_w	recirculation length

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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_∞	free stream Pressure
$\overline{PN}$	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 diferencing schemes or grid refinement ratio
Re	reynolds number
R_c	radius of curvature for bend
$\mathbf{S}$	deformation rate (strain-rate) tensor or surface area vector or symmetric part of the velocity gradient
St	strouhal number
S_p	linear part of the source term
S_u	constant part of the source term
S_ϕ	source term
t	time
$\mathbf{u}$	velocity vector
u	velocity magnitude
$\mathbf{u}_c$	relative velocity
V	volume
ω	vorticity
(x_a, y_a)	coordinate at front of cylinder
(x_e, y_e)	coordinate at end of cylinder

Greek

α	VOF color function
$\alpha_{\max}$	maximum value of color function
$\alpha_{\min}$	minimum value of color function
Γ	interface or difusivity
γ	forcing function constant
δ	curvature ratio of the tube bend
Δ	difference
Δt	time step size
Δt_{max}	max time step
ε	turbulent energy dissipation, Penalization parameter
ζ	damping coefficient
η	forcing function constant
θ	angle or leaflet's angle
θ_s	separation angle
κ	Interface curvature or bulk viscosity
λ	lagrange multiplier or tensor eigenvalue
λ_2	second invariant of tensor
λ_1, λ_2	adaptive time step coefficient

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μ	dynamic viscosity
μ_f	fluid dynamic viscosity
μ_s	solid dynamic viscosity
μ_t	turbulent dynamic viscosity
μ_{SGS}	eddy viscosity
ν	kinematic viscosity
ρ	density
σ	surface tension
τ	shear stress or period of vortex shedding
τ_w	wall shear stress
τ_{eq}	equivalent shear stress
τ_e	stress tensor for hyperelastic material
ϕ	general scalar property
ξ	moment around the hinge axis
Ω	antisymmetric parts of the velocity gradient
Ω_f	Continuous of fluid domain
Ω_s	embedded or solid domain
ψ	TVD limiter
Ω_1	continuous domain properties
Ω_2	embedded domain properties

Superscripts

'	fluctuating component
T	transpose
α	model constants for BDI
β	model constants for BDI
n	discrete time level
L	linear term for the flux F
NL	non-linear term for the flux F
$\bar{\phi}$	filtered variable

Subscripts

(i,j)	(x,y) cell coordinates
x, y, z	coordinate components
f	face interpolation
N	neighbouring cell N
P	owner cell P
SGS	turbulent SGS properties

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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 ofblood clotting. However, if a blood clot develops in a patients 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 a 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 Vincis 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.

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Figure 1.1: Similar pattern between postulated (da Vinci's) and measured blood vortices in the aortic root
(Source: Bissell et al., 2014)

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). Its 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.

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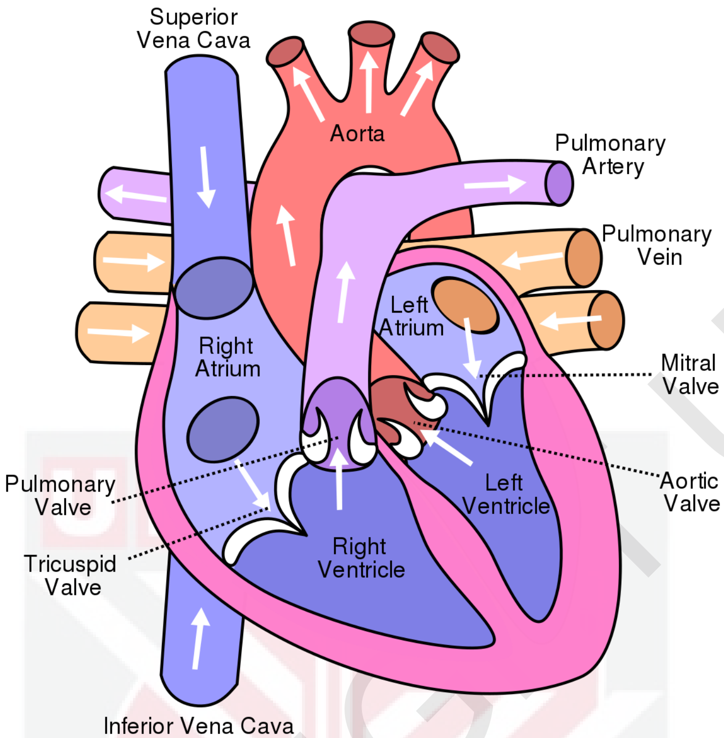

Figure 1.2: Direction of blood through the valves

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

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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 α 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.

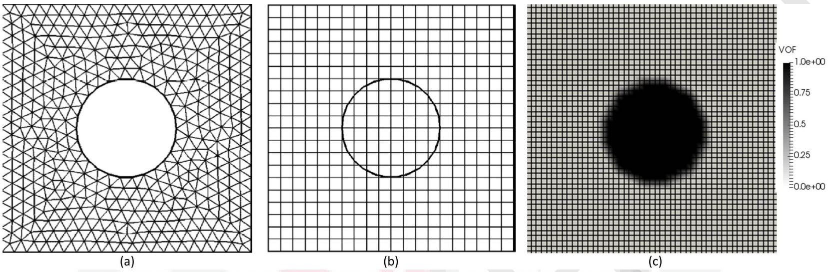

Figure 1.3: Schematic view comparison of grid structure between (a) BF, (b) NBF and (c) VOF methods

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 as 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 μ and colour function α 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 reseach direction on numerical method, and aerody-

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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

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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.

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