Marcin Nowak

Development of numerical model for modeling artificial heart valves for performing virtual therapies

PhD thesis

Supervisor:
Wojciech Adamczyk, PhD, DSc, Assoc. Prof.
Co-supervisor:
Eduardo Divo, PhD, Prof.

Silesian University of Technology

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Extended abstract

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Aortic valve disease is one of the most common cardiovascular disease. This group is the leading cause of death in the modern world, and according to the World Health Organization, they was responsible for 31% of deaths in 2015, and in Europe 45% of all diseases are their consequences. The cardiovascular pathological changes lead to the common diseases, such as atherosclerosis, aneurysm, stroke, heart attack and valvular diseases. The last group can be divided into congenital defects, such as biscupid aortic valve, or they appear as a disease with aging. The most common valvular disease is calcified aortic valve disease, reaching 13% in the general population over 65 years; without proper treatment, 80% of patients suffer heart failure or mortality five years after diagnosis. For patients with advanced calcification stage, artificial aortic valve implantation is the only option, however this can lead to medical complications. Commonly used mechanical valves increase the risk of thrombosis, infection, paravalvular abscess, or perivalvular leakage and require constant anticoagulation therapy. Bioprosthetic valves (artificial or animal) are prone to deterioration and have limited durability. An ongoing task in the medicine and engineering is to reduce the mortality on the civilization diseases and improve society's life. There is a large potential in the development of a hybrid approach that combines fast echocardiography with an advanced numerical model developed in the framework of computational fluid dynamics. However, it is important to use in a clinician practice a robust, reliable, error-proof and validated computational models. Numerical modeling has had various applications, and they are divided in two categories: cardiac models, and vascular models. The model validation can be performed with the use of the laboratory test rig measurement data and also using the patient-specific data coming from their medical examination, where

in this Ph.D. thesis both pathways were utilized. The measurement data were gained from the inhouse laboratory test rig, located at Department of Thermal Technology, Silesian University of Technology, whereas the medical data were accessed from the available literature. The goal of the Thesis is to show the feasibility and validity of the different approaches for the modeling the movable, rigid and deformable structures, as human and artificial valves. The models were analyzed also in terms of their computational efficiency, for the implementation towards the virtual therapies. Different moving mesh approaches were used and their results and validity were compared.

The complex problem of the blood flow through the rigid-rotary or flexible structures, required a usage of the expanded mathematical models. This comprise the solving of the physics present on the fluid and the solid side, also the interaction between those two participants. The fluid equations included the partial-differential Navier-Stokes equations, turbulence model and Windkessel model for outflows, created based on the electrical analogy. Also, the non-Newtonian viscosity model had to be implemented into solution procedure, if the blood flow was analyzed. On the solid side, the structural governing equations were applied, which allowed to calculate the transient deformation fields. For the rigid bodies, the inhouse model was implemented into the fluid solver to determine their motion.

Solving of the Navier-Stokes partial differential equations (and other, related e.g. to the turbulence, hemolysis or cavitation) using CFD software, enables the determination of the flow conditions. The geometry of the fluid or solid domain, gained by patient examination (e.g. magnetic resonance imaging) or created using computer aided design software is discretized, and the numerical method is applied to solve equations within the domain. Blood is a mixture of plasma and blood cells, however it can be treated as a single non-Newtonian fluid, which means the non-linear dependence between shear stress and shear rate. The solid properties of the blood tissue have to be known, to properly solve the deformations which result from applied forces, coming from the flowing blood. The aorta walls, as well as aortic valve leaflets, are multilayer structures, anisotropic, viscoelastic and also hyperelastic. Such properties are modeled by applying constitutive material model, as Hookean or Mooney-Rivlin, which express the strain energy density function from the deformation tensor. Generally, the blood tissue is highly elastic and deforms due to relatively small forces that act in the cardiovascular system due to the flow of blood and the movement of the human body.

The interaction between the physics present on the fluid and solid side, is modeled via applying Fluid-Structure Interaction technique. Many different approaches to model FSI are present, as the rigid body solver (as implemented in this thesis for artificial valve), partitioned with two separate solvers (for fluid and solid) and monolithic, where both the fluid and solid equations are solved in single monolithic matrix. The comparison of different FSI modeling approaches and software can be found in *Konstantinos G. et al, Comparison of numerical implementations for modelling flow through arterial stenoses. IJMS 2021.* Furthermore, the comparison of the FVM and FEM for FSI, to the results of the computational model can be found in *D. Lopes at al, Analysis of finite element and finite volume methods for fluid-structure interaction simulation of blood flow in a real stenosed artery. IJMS 2021.* The partitioned approach can be utilized as one-way or two-way coupling. The first is valid when the influence of solid deformation on the flow field is negligible, so the deformations are low. Therefore, the coupling procedure is realized only once, i.e. the results from steady-fluid solver are transferred as the boundary condition to the structural solver. In the second approach, i.e. two-way coupling, the transient flexible body motion is captured, and multiple coupling procedures are performed during every timestep, till both solvers and transferred values (force and displacement) are converged. This approach was used in this investigation to model the anatomical aortic valve.

Numerous applications of the modeling are found for the anatomical and artificial valves, e.g., for the assessment of the disease severity, investigation of the calcification process, diseases formation and prevention, and also for prostheses design. However, there is still room for improvement in the design of prostheses and also in the modeling approach itself, which could improve the applicability of modeling for medical practice and may contribute to the progress of therapeutic outcomes. Different approaches can be found for FSI, and the choice depends on the level of fluid-solid coupling, geometry complexity, deformations, and computer resources. For example, the partitioned approach includes two separate solvers (fluid solver and mechanical solver) and a module that couples each other. Such an example usage can be found in *A. Amindari* *et al, Assessment of calcified aortic valve leaflet deformations and blood flow dynamics using fluid-structure interaction modeling. IMU 2017*, where a computational model was applied to predict the impact of the calcification process on the hemodynamics of the aortic valve, including pressure drops and flow patterns. Research *Loureiro-Ga M. et al, Including coronary ostia in patient-specific 3D models of the whole aortic valve apparatus, derived from TEE, for biomechanical simulations. Int Jnl of Multiphysics 2021* presents a semi-automated numerical modeling process that considers the aortic valve, left ventricle, and coronary ostia. 3D-TEE image sequences (Transesophageal Echocardiography) were used for automatic CAD geometry and mesh preparation. The COMSOL® Multiphysics *(https://www.comsol.com/comsol-multiphysics)* was used to solve the FSI phenomenon, using *monolithic approach*, suitable for large deformations. The procedure using a strongly coupled 3D FSI model for transcatheter aortic valve replacement, interacting with complex valvular, ventricular, and vascular disease, was presented in *Khodaei S. et al, Towards a non-invasive computational diagnostic framework for personalized cardiology of transcatheter aortic valve replacement in interactions with complex valvular, ventricular and vascular disease. IJMS 2021.*

The Ph.D. study was divided into six chapters and three appendices containing source codes used in the Fluent journals and UDFs, as well as the Python source codes used for the image processing programs.

Introduction chapter includes information on the necessity of biomedical engineering development, in terms of the high clinical demand for computer algorithms. The diseases of the aortic valves and prostheses used for human valve replacement are described. Anatomical build, mechanical characteristics and operation of the human valve is also described. The basic concepts regarding computational modeling methods for fluid, structural and FSI solvers are explained. The literature review shows the current stage of knowledge in terms of computational modeling and laboratory measurement, applied for vascular CFD and FSI, especially for valve modeling. The author's experience with cardiovascular modeling and laboratory test-rig measurement was outlined.

Mathematical model describe the physics in terms of the fluid, structural, and FSI coupling equations, built-in the commercial Ansys® software. In addition, the mathematical approach for internal algorithms is described here. The equations for turbulence models are described. The electrical analogy model for the outlet boundary condition is presented. The inhouse model and mathematical expressions for determining rigid body motion, and dynamic time step size for the solver, is described, with its application for the mechanical valves. The partitioned fluid structure algorithm for anatomical valve is described, where the fluid *Fluent* and structural *Mechanical* Ansys solvers were used. The solution workflow is presented graphically in the flowcharts. The material model for the non-Newtonian Carreau viscosity is presented. The applicability of the models used is described. Information regarding the geometry discretization into numerical mesh, and the moving mesh approaches and applications is described. The guidelines for discretization preparation in order to avoid possible problems, as negative cell volume or orphan cells are presented. The basic indicators on human and artificial valve performance, used in the following chapters, are described here.

Artificial valve modeling is described in Chapter 3. The artificial bileaflet valve was virtually implanted within the geometry of the real patient, containing the aortic root, the ascending and descending aorta, and the main arterial branches. The different Reynolds-averaged Navier–Stokes (RANS) turbulence models were applied to assess their validity and applicability for valve modeling. The valve motion was imposed using the measured angular profiles found in the literature. The lumped-parameter model for the outlets was applied here and the results were compared with the simpler 0 Pa gauge pressure boundary condition. The impact of limited usage of the geometry scope on the results was assessed. The geometry processing of the magnetic resonance angiography model, and mechanical valve leaflets, is described, also the preparation of the overset numerical mesh usage is presented.

Extension of the FSI approach for the mechanical valve with validation is described in Chapter 4. The laboratory test setup and equipment is presented for the validation of the models. The in-house 6DOF model is presented to be time-efficient for the rigid rotating structures. The novel approach to dynamic time-step sizing is implemented in the solution procedure, which considerably improved moving mesh operation, solver convergence, and computational efficiency. The model was validated using an in-house test rig managed by the Labview application, equipped with the pulsatile blood pump, fast camera, mass flow meter, pressure transducers, and valve holder designed for the measurements. A data set was used for the model calibration, i.e. the moment of inertia constant, and four validation datasets confirmed the excellent model validity, based on the valve leaflet angle courses and pressure values. The in-house Open Source Computer Vision (OpenCV) algorithm was developed to process the fast camera images into leaflet angle values. The model results involving the overset moving mesh method were compared with other moving mesh approach, i.e. dynamic mesh of three different approaches. The stability, validity and preparing process of applied moving mesh modules is compared.

Modeling anatomical and artificial aortic valve stenosis is described in Chapter 5. The application of the novel, advanced moving mesh model, which consists of the coupling of the dynamic mesh smoothing and the overset mesh technique, to speed up the FSI computation and improve the convergence and stability was shown. Real 2D and 3D vasculature and valve geometries were created based on the echocardiography images available in the literature. The calculations of anatomical and artificial valve models were performed for the various severity of the atherosclerosis, not previously published for the mechanical valve. The impact of the calcification process on natural and artificial aortic valves was assessed and compared. The sensitivity of the mesh density onto deformation and pressure solutions is verified. Two solid material models: Hookean and Mooney-Rivlin, were used and compared based on the valve leaflets deformations. The validity of the rigid aorta wall assumption was assessed, and the aorta wall time-varying deformations are presented. The validation of numerical model results was performed based on the literature measurement data, which included the valve shape, velocity pathlines, pressure drop values and valve opening. The computer vision protocol for determination of the elastic valve opening based on the large set of images was described.

Discussion and conclusions chapter summarizes the conclusions derived based on the research carried out, and indicates the topics that researchers should consider in the future in terms of vascular CFD and measurement.

The thesis presented the development of numerical models for the modeling of artificial and anatomical heart valves, applying to rigid and deformable. The comprehensive analysis was performed for accurate, robust, stable, and time-efficient computations, which included selection of an efficient computational strategy, development of an in-house model for modeling fluid-structure interaction, and definition of the geometry, mesh, and proper timestep size of the solution procedure. The in-house model was dedicated for the accurate time discretization control in the transient model, for efficient and reliable application of the moving mesh modules. All mentioned aspects characterized the numerical model in the case of its usage for clinical diagnosed trials, in consideration to support the patient examination, for example for virtual therapies. Implementation of the module calculating timestep size appropriate to the determined leaflet velocity improved considerably the solver stability, moving mesh operation, and significantly reduced solving time by 72%. The overset mesh approach turned out to perform better in terms of computational efficiency, as the smaller rotations per single timestep were demanded for the dynamic mesh module used instead. The in-house 6DOF model proved to be quite insensitive on momentum of inertia error, cause the value change on the level of ±40% did not influence significantly onto the valve leaflets angular motion, also even with less impact on other CFD characteristics. The CFD results and determined valve indicators shown a proper valve operation, confirming the conclusions made based on the real arterial geometry model with virtually implanted valve. The approach for modeling deformable valve prostheses was also recognized and implemented, both for the 2D and 3D elastic valve model. The author experience *(Nowak M. et al, The protocol for using elastic wall model in modeling blood flow within human artery. Eur. J. Mech. B Fluids 2019)* of the arterial flow FSI modeling was transferred to the flow-around modeling of the deformable valve. Using the remarks made on the moving mesh approach for the rigid valve and flexible aorta, the novel approach combining two modules, namely dynamic mesh and overset mesh, was applied for the flexible leaflets structure, which improved considerably the moving mesh quality, solver stability, boundary layer resolving and solving time. The procedure for using such coupled meshing module was described, both for the 2D and 3D geometries, along with the mesh testing procedure omitting flow and structural field resolving. The partitioned FSI approach combining the fluid and mechanical solver, was used for the anatomical valve, where to compare its operation with the prosthesis, the validated 6DOF model was successfully applied for the bileaflet valve. The flexible valve model demanded tremendous computational resources, therefore the full 3D geometrical model was reduced to 2D approach. However, the opportunities for solving the model in 3D coordinates were recognized and described. The declining inflow rate provoked anatomical valve closing for all the calcification stages, where the reversed flow have to be present to provoke the mechanical bileaflet valve closing. Similar opening and closing times are determined for the human and artificial valve. Slight fluctuations in terms of the rigid leaflets angular position and flexible leaflets deformations are present during the valve opening and closing phases. Based on numerical model results, calcification of the human aortic valve change its kinematics more in terms of the maximum opening (35.9% decrease for the severe calcification), than for the maximum closing (approximately equal 5% decreases in closing for all calcification stages). The healthy artificial valve causes less maximal pressure drop (240 Pa) than the anatomical valve (850 Pa). TPG values rised due to valves calcification. The eddy structures are more prominent for the anatomical valve due to its curved leaflet shape. The bileaflet valve produces regular, three-jet flow, however vorticity is still present, especially in the sinus regions, starting from the moment when the velocity decreases. Blocking of the one mechanical valve leaflet, at its closed state, caused by sticking to the arteriolosclerosis plaque, provoked several time increase in the TPG and WSS values exerted on leaflet wall. Slightly higher WSS values were noticed for the bileaflet valve, WSS values rise due to the stenosis. The stenosis increases the vorticity magnitude for the anatomical valve by several percents, where for the mechanical valve a progressive decrease by about 3% per each calcification stage is noticed.

The topics for the future research are presented. As indicated in the review of the literature and based on the conducted research, there is still room for improvement in terms of the artificial valve design, both for rigid and deformable valves. The construction should overcome drawbacks in terms of the possible high shear stresses causing blood cell lysis, high rotational speed that may cause cavitation bubbles, high pressure drops and resulting flow obstruction, durability problem of the elastic valves, also its interaction to the blood walls and overall circulatory system. The developed 6DOF-FSI and

FSI validated models can be successfully used in multivariant analyzes, which will support the decision-making process on the best design for the specific patient's conditions. The parameters related to the geometry, influencing the valve operation, are for example the leaflet length (rigid and deformable valves), angular position limitations and location of the rotation center (rigid valve), number of leaflets, leaflet thickness, and material properties. The impact of these parameters values onto prosthesis operation will be analyzed in the future work. The artificial intelligence, multiphase and blood cell lysis models, also the open-source solvers will be used in the future research concerning aortic valve, cardiac and vascular numerical modeling.