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Review of a doctoral dissertation of Marcin Nowak, MSc, "Development of numerical model for modeling artificial heart valves for performing virtual therapies"

The review was prepared at the request of Prof. Marek Gzik, PhD, DSc
included in the letter sent to me of June 2, 2022.

1. Overall assessment.

The subject of the thesis concerns numerical modelling of Newtonian and non-Newtonian flows in artificial aortic valves. The work focuses on the use and adaptation of commercial ANSYS software and university software to solve an important engineering problem. **In my opinion, the subject of the thesis and the methods of analysis of the issues considered in it allow qualifying this thesis for the discipline of biomedical engineering.**

The main goal of the work was to create a simulation methodology and a numerical tool that allows for CFD modelling of blood flow in the human circulatory system in the vicinity and through aortic heart valves, taking into account the movement of their blades and tissue deformation. Due to the specificity of the issue, conducting experimental research on a real "object under working conditions" is extremely difficult and requires the use of non-invasive measurement techniques based mainly on the imaging of the flow field and deformation of soft tissues. This makes the available experimental results often imprecise and incomplete compared to the results typically obtained in research on flow problems. Moreover, the results of this type of research are difficult to generalize due to the uniqueness of the "research object".

The thesis implicitly puts forward that the use of modern CFD methods for this purpose will allow for an in-depth analysis of the flow field and tissue deformation and will enable the assessment of the effectiveness of heart valves in various conditions.

The work focuses mainly on related technical issues with the creation of various types of computational grids, the algorithm determining the movement of the valve blades and comparisons of various variants of flow field modelling methods. Less attention has been paid to the effectiveness and correctness of valve operation. The methods adopted for the description of the work performed, the analysis of the results as well as their presentation and verification using the available experimental data are correct. **The work is original and presents the degree of complexity customarily found in doctoral theses. It was carried out as part of the NCN and NCBiR projects.**

2. Detailed assessment.

The thesis was written in English, thanks to which it can serve as a scientific aid to a wide group of scientists. The layout of the work is typical to the one I have encountered so far in the doctoral dissertations reviewed by me. Its main part consists of an introduction, four chapters describing the mathematical model, the results of verification of the performed simulation, the results of comparisons of the flow fields through the anatomical and artificial valve, and a summary. The list of literature is very extensive and contains 169 references, including 6 items co-authored by the PhD student. The cited articles are up-to-date and published by recognized publishers. The paper also includes three appendices, which present two scripts prepared by the PhD student in Python for the analysis of the position of the valve blades based on pictures/photos, and the UDF (User Defined Function) script that defines the change of the computational grid during the movement of the valve blades.

The literature review presented in the introduction is very extensive. It shows the current state of knowledge on the use of heart valves, related problems and the methodology of research aimed at their improvement and analysis of the effectiveness of the operation. The introduction also presents the scope, purpose and summary of the work carried out as part of this doctoral dissertation. In my opinion, some information is unnecessarily repeated in subsequent subsections, which gives the impression that some fragments of the work were directly transferred from previous reports or articles of the PhD candidate without taking into account the fact that the information has already been given. This remark also applies to the following chapters, but it does not diminish the substantive value of the work.

In the simulations performed, the 6DOF program and the ANSYS program were used with prepared UDF procedures. Chapter 2 presents two types of computational grids used for geometry changing over time, the so-called overset mesh and dynamic mesh. After reading this part of the work and the detailed descriptions of this issue in the following chapters, I have no doubt that the PhD candidate has a lot of knowledge and practical skills in this topic. Chapter 2 also presents the mathematical model of fluid motion. After reading this fragment of the work, I came to the conclusion that it would be better for the PhD candidate to skip this issue and briefly write what models he used. There are many errors and inaccuracies in the formulas presented by the PhD candidate. For example, should the variables that define density, time, and viscosity in equations 2.1-2.2 not be the same as in equations 2.12-2.13? It is not true that in an incompressible flow the derivative of the density over time is zero, this is the case only when the density is constant, and it does not have to be that in an incompressible flow. Where are the formulas 2.7 and 2.8 used? In equation 2.9, the index of the sum in the denominator is incorrect. How should it be understood that the solution of a non-conservative form of the equation is not a problem when the solution is convergent. Does it mean that even if the solution converges, for example without the condition of mass conservation, it is correct? In the definition of the Reynolds number in 2.3 the variable 'd' is generally a characteristic dimension, not necessarily a diameter, and the variable 'u' is a modulus of velocity, not velocity. How turbulent viscosity is defined in the equations 2.12-2.13? In equation 2.14, the symbol \eta is defined. Is that correct? After all, \eta is used as viscosity in the definition of the Reynolds number. Lack of uniformity in the notation! Do the velocity components appearing in equation 2.15, written in capital letters, mean the velocities are different than those in the other equations? In equation 2.15, \Omega should have indices 'ij'. What are the Prandtl numbers in the equation 2.12-2.13 and 2.16-2.17? By the way, 2.16-2.17 are not the equations for "model constants" as written in the line above. How is it to be understood "y is the gradient in streamwise velocity in the direction perpendicular to velocity"? Chapter 2.5 deals with a very important issue, i.e., the boundary conditions at the outflow, which has received a lot of attention in the thesis. I do not understand how equation 2.19 was obtained from 2.20. It does not seem as trivial as one might conclude from the presented description. Chapter 2.6 presents the algorithm of the 6DOF program for the analysis of the fluidsolid interaction. How should the phrase "Second, it was not clear to us ..." be understood. What "us" did the PhD candidate have in mind. Equations 2.22 and 2.23 do not lead to 2.24. What does "body's momentum of momentum" mean? Equation 2.27 (lack of module sign in the first segment), which is treated as one of the innovative elements of the thesis, was derived from 2.26. This was only possible under the assumption that the time step is positive, otherwise, it could not be taken out from the module sign in 2.26. Solving the equation (not the function as written in the paper) provides two solutions for the time step: positive and negative. Does the PhD candidate not see a certain inconsistency here? In equation 2.34, there is a variable \omega that previously stood for angular velocity and so it is written in the list of symbols. This time it means a relaxation coefficient. If it is equal to 1, as written, it would be better to omit this term completely than to do a mess with the symbols. The \phi variable with 'curr' and 'prev' indexes does not mean the current and previous iteration, but the value \phi in the current and previous iteration. There are a few more bugs similar to those listed above, ambiguities also in wording, also later in the work. In general, I believe Chapter 2 was written carelessly and as if in a hurry to copy equations from various sources. However, I believe that such errors did not occur in the scripts prepared by PhD students.

Chapter 3 deals with modelling the flow through an artificial aortic valve. A lot of attention was paid to the methods of generating the computational mesh. This is a well-written chapter of the work. Please let me know if the wall functions (which) were used in the simulations and what was the y+ parameter when using 7 layers of near-wall cells.

Figure 3.5 shows a comparison of the simulation results obtained without the turbulent flow model and with the two previously described models on 3 computational grids with different numbers of nodes. It shows that the "medium" mesh provides results that are practically independent of the number of nodes. Please present the comparison of the results on one graph obtained on the "medium" and "fine" grids without the turbulent flow model and with two models. Please present the spatial and temporal variability of the turbulent viscosity. This will show whether the use of the turbulent flow model makes sense, and it will be more reliable than the argumentation based on the results shown in Figure 3.10, which erroneously shows that the local Reynolds number is the largest near the walls. Well, with the Reynolds number defined on the basis of the equivalent diameter and mean velocity, Fig. 3.10 shows only the trend of viscosity variation determined from 2.18. It is the largest near the wall where the stresses are the largest. Please correct me if I am wrong. Chapter 3.3 is devoted to the model settings. Please let me know why to solve 2.19 it was necessary to use the RK method of the 4th order. By the way, the phrase "O (h^5) is called 4-th order error" is wrong. This is an error of the 5th-order RK method. Therefore, it is said that the RK method defined by 3.1 is 4th order because it is consistent with the 4th order terms of the Taylor series. Please let me know how TKE was determined in J/m^3 when defining TKE (3.3) in m^2/s^2. In the line above Fig. 3.11 there is an incorrect reference to 4.15. In fig. 3.13 there is no "red curve" in my version of the thesis. Nevertheless, the result presented on it is very interesting and important. It shows where recirculation areas are formed and where, and in which phase of the flow high the shear stresses can be expected and destroy the blood cells.

Referring to Fig. 3.15, cavitation is mentioned. Would expect the cavitation based on the presented results? I do not understand why discussing these results presented in Pascals, then the discussion is continued (p. 73) based on mmHg. Did I miss something in between these parts of work? Similarly as in fig. 3.15, it would be good to show how the maximum stresses change on the valve blades. Surprisingly small are the differences in the simulation results for the case with/without the valve, shown in Figs. 3.18 and 3.19. Please explain why this is so. Chapter 4 concerns the development of the FSI model for the needs of flow analysis through a mechanical valve and its verification based on the conducted experimental studies. As before, I am asking for the y+ value in the simulations performed. In Fig. 4.1D, the marked angle is rather not equal to 25deg. Overall, the chapter is well written and the research presented in it must have taken a lot of work. In my opinion, the obtained simulation results agree very well with experimental data, which confirms that the procedures prepared by the PhD student are free of "large" errors. The conclusions from the comparisons of the simulations made on the overset and dynamic mesh are very interesting and a bit surprising.

Chapter 5 is devoted to the analysis and comparison of flow in a valve with an anatomically deformable shape and an artificial valve with regard to several phases of calcification. This is a very valuable piece of work, although, due to computational costs, most of the calculations were based on the 2D model. I do not understand the information that "The artificial valve geometry was created based on the user manual." The simulation results agree well with the experimental data (Figs. 5.11 and 5.12). Very interesting is the result showing that to close the anatomical valve is enough to slow down the flow, while to close the artificial valve a backflow is needed. Please present Figure 5.16 in the same colour scale on the left and the right side of the individual subfigures.

The thesis ends with a summary that accurately describes the scope of the research and the results obtained, and indicates future directions of work.

Reading this thesis brings me one more question. The simulations took into account the influence of the flow field on velocity, deformation and valve opening. Why did the simulations not take into account the effect of the elasticity of the valves that affect the fluid when they close? I have drawn this conclusion on the basis of the description of the model in which there are no terms responsible for this type of interaction.

The thesis is written clearly and communicatively. I noticed quite a lot of linguistic mistakes, but the text is understandable and will be legible both for "native speakers" and for other people. There is no way in which these types of mistakes, which unfortunately most of us make, do not affect my substantive assessment of the work. The errors in the description of the mathematical model, which I wrote about in the review, I suspect that they resulted not so much out of ignorance and carelessness of the PhD student, but in a hurry due to the deadline for submitting the thesis. **Undoubtedly, the presented work is positive proof of the knowledge and skills of the PhD candidate. The results obtained by him and the prepared software constitute a valuable contribution to the development of CFD methods.**

3. Conclusion

To sum up, the dissertation presented for review is, in my opinion, a solution to a complex scientific task. PhD student made an original contribution to the development of computational fluid mechanics tools. The methods and numerical tools prepared by him will certainly be used in the future, and the obtained results are of great cognitive value. This allows to state that the assumed goals of the work have been achieved. The presented doctoral dissertation proves the knowledge of the PhD student in the field of numerical modelling of flows and the use of commercial computational tools, and confirms the ability to independently conduct scientific research. Taking the above into account, I conclude that the doctoral dissertation M.Sc. Eng. Marcin Nowak meets the requirements of the Act on Scientific Degrees and Title and I am asking for the thesis to be admitted to public defence.

Tyliszczak A.

Prof. Artur Tyliszczak