Jan Oldenburg*, Julian Renkewitz, Michael Stiehm and Klaus-Peter Schmitz

Contributions towards Data driven Deep Learning methods to predict Steady State Fluid Flow in mechanical Heart Valves

Abstract: It is commonly accepted that hemodynamic situation is related with cardiovascular diseases as well as clinical post-procedural outcome. In particular, aortic valve stenosis and insufficiency are associated with high shear flow and increased pressure loss. Furthermore, regurgitation, high shear stress and regions of stagnant blood flow are presumed to have an impact on clinical result. Therefore, flow field assessment to characterize the hemodynamic situation is necessary for device evaluation and further design optimization. In-vitro as well as in-silico fluid mechanics methods can be used to investigate the flow through prostheses. In-silico solutions are based on mathematical equations which need to be solved numerically (Computational Fluid Dynamics – CFD). Fundamentally, the flow is physically described by Navier-Stokes. CFD often requires high computational cost resulting in long computation time. Techniques based on deep-learning are under research to overcome this problem. In this study, we applied a deep-learning strategy to estimate fluid flows during peak systolic steady-state blood flows through mechanical aortic valves with varying opening angles in randomly generated aortic root geometries. We used a data driven approach by running 3,500 two dimensional simulations (CFD). The simulation data serves as training data in a supervised deep learning framework based on convolutional neural networks analogous to the U-net architecture. We were able to successfully train the neural network using the supervised data driven approach. The results showing that it is feasible to use a neural network to

estimate physiological flow fields in the vicinity of prosthetic heart valves (Validation error below 0.06), by only giving geometry data (Image) into the Network. The neural network generates flow field prediction in real time, which is more than 2500 times faster compared to CFD simulation. Accordingly, there is tremendous potential in the use of AI-based approaches predicting blood flows through heart valves on the basis of geometry data, especially in applications where fast fluid mechanic predictions are desired.

Keywords: Mechanical Heart Valve, Convolutional Neural Network, Deep Learning, Fluid Flow, Computational Fluid Dynamics

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1 Introduction

Cardiovascular diseases rank among the most common diseases with high mortality in industrialized countries (Germany: 20.4 deaths per 10,000 patients) [1]. In particular, aortic valve stenosis and insufficiency occur due to high flow and pressure conditions. Besides reconstruction, the treatment of choice is valve replacement using heart valve prostheses (aortic interventions Germany: 30.838) [1]. It is commonly accepted that among other factors, the long-term outcome of aortic valve replacement depends on their hemodynamic performance. In particular, aortic valve stenosis and insufficiency are associated with high shear flow and increased pressure loss [2]. Furthermore, regurgitation, high shear stress, and regions of stagnant blood flow are presumed to have an impact on the clinical result [2]. Therefore, the analysis of the velocity field is of high interest. In-silico methods have been established in the past, but show limitations in terms of computational effort when it comes to fast design optimizations or patient individual decision making based on flow fields.

In recent years, artificial intelligence, especially deep learning, has made tremendous leaps forward. In particular,

***Corresponding author: Jan Oldenburg:** Institute for ImplantTechnology and Biomaterials e.V., Friedrich-Barnewitz-Str. 4, 18119 Rostock-Warnemünde, Germany, michael.stiehm@uni-rostock.de,

Julian Renkewitz: Student of Institute for Biomedical Engineering, Rostock University Medical Center, Rostock-Warnemünde, Germany

Michael Stiehm, Klaus-Peter Schmitz: Institute for ImplantTechnology and Biomaterials e.V., Rostock-Warnemünde, Germany

this progress is driven by image recognition and analysis and has achieved good results in radiology problems [3]. In fluid mechanics, the use of deep learning is also being investigated. For example, Seka et al. [4] have used convolutional neural networks to estimate fluid flow patterns around airfoils. In this study we apply a related concept to estimate the flow through aortic root geometries with implanted mechanical valve prosthesis. Here, we follow a data-driven deep learning approach for which training data is required. Computational fluid dynamics simulations based on the Navier-Stokes equations, numerically solved using Finite Volume Methods, will be used as training data.

2 Materials and Methods

The following steps need to be made to get to a supervised data-driven trained neural network for estimating fluid flow through aortic root geometries with mechanical heart valves implanted. At first, random generation of aortic root geometries. Second, the geometry data will be simulated. Third, the CFD - simulation data will be converted to image format for use in deep-learning environments. And fourth the training and validation of the neural networks will be performed.

2.1 Aortic root geometries

We used MATLAB to create random, individual aortic root geometries (STL file). For two-dimensional mapping of the aortic geometry, annulus diameter (corresponding to valve diameter) of 20 mm, 24 mm, and 28 mm were chosen. We assigned random variables to the position of the inversion point in the sinus. To improve the reconstruction of an aortic root from these concise anatomical points, randomly supporting points were generated. The point-intervals were defined according to the typical minimum and maximum values given in the literature [5-9]. The *pchip* function in MATLAB was used to interpolate the points, which are different for each case.

Figure 1: Schematic representation of the ascending aorta with mechanical heart valve. a) 3D view and b) 2D view; The ascending aorta simplified consists of the annulus plane with the mechanical valve, the aortic sinus Valsalva and the junction between sinus and tubular part of the ascending aorta.

The geometry of the mechanical valve (comparable to the St. Jude) is represented in a simplified way by using rectangles, which have a length corresponding to the diameter. The angle between both wings measured 120° when closed. The thickness of the flaps is fixed at 1 mm. The idealized valve geometry was also saved as STL file format.

2.2 Computational Fluid Dynamics

Due to the complex 3-dimensional structure of the anatomical aortic root, the flow can be considered as 3-dimensional. Nevertheless, some working groups have performed 2-dimensional simulations [10, 11]. The simplification to 2-dimensional simulations should be discussed. Here, to reduce the computational effort, we have performed the CFD simulation in two dimensions as well as under steady state conditions. The simulations were performed with the open-source software package *OpenFoam*. We used *SnappyHexMesh* to insert the aortic root geometry and the valve into a pre-generated blockwise mesh (using *blockmesh*). For simulation, we chose the steady state solver *SimpleFoam* and implemented a k-epsilon RANS turbulence model. The final mesh has a refinement of more than 155,000 cells. 3,500 simulations were performed using a batch scripted process. Convergence of the solution was reached in about 30 min using a Xeon E5-2640 v3 (2.6GHz).

2.3 Prepare Data for Training

Simulation data and input data are processed using a custom-made MATLAB script. Many deep-learning algorithms are specialized for image data. The input geometry is the calculated Euclidean distance of each pixel to the fixed pixelated walls. The corresponding CFD-Simulation was interpolated to an image like fixed grid. The prediction of the neural network is also in form of an image featuring two channels (U, V). Data was rescaled between [0, 1] according to monitored maximum and minimum velocity values.

2.4 Neural Network Design and Training

We used two neural networks comparable with the U-net network. This network has a down convolution path and an up-convolution path with skip connections. The first network is a classical U-net network and the second is an U-net with dense connections in the layer with most features. As input, we have the Euclidean distance boundary representation of the aortic root. The network will generate an output showing the predicted steady-state flow through the mechanical heart valve. We performed training of the neural network using

TensorFlow 2.0. For training, we have a total of 3,000 CFD-Simulations. To perform training and optimize the weights of the neural network we used the adaptive momentum optimizer (Adam learning rate: 0,001) and a batch size of 10. We performed weight optimization for 300 Epochs (One Epoch = all training data processed). The Loss that will be reduced is the pixel-wise averaged mean squared error between prediction and simulation. The training was performed on a GPU (Quadro M5000) with a total training time of 3.5 hours.

For Validation of the network, 90 Simulations were used that were not included in the training of the neural network. We used the Mean Squared Error of the network prediction concerning the validation data.

3 Results and Discussion

We used supervised learning to train two neural networks. A set of 3500 CFD simulations were used as training data. Based on 90 unseen aortic root geometries, we carried out validation by estimating the Mean Square Deviation pixel-wise from performed CFD simulations (interpolated to image coordinates corresponding to the AI results) and the estimates of each trained neural network. The 90 unseen geometries include 3 different valve sizes. Shown are valve size 19 mm (green) and 29 mm (black), which are outside of the valve size range used for training, and 24 mm (magenta), which is inside of valve size range used in training.

Figure 2: Prediction error (mean squared error) during training on unseen training data of two neural networks (Unet and Unet + Dense). Shown are: valve size 19 mm (green) and 29 mm (black) - outside of valve size range used for training and 24 mm (magenta) - inside of valve size range used for training.

Figure 2 shows the deviations by the number of training epochs. From 100 epochs onwards, no improvement of the deviation is noticeable, even with unseen valve sizes. Both neural network architectures work well on valve sizes which lay in between seen sizes in training. For valve sizes outside the training size range, U-net with dense connections works better.

3.1 Network Prediction Performance

To get a better qualitative impression of the performance of the networks in comparison with CFD data, the estimated velocities (U, V) and the pressure (P) are compared with the CFD result on a representative aortic root geometry. Both neural networks show a physiological flow pattern with small deviations to the CFD.

Figure 3: Fluid flow prediction on unseen geometry data using two different neural networks compared with CFD-simulation results. The velocity in x- and y-direction are color scaled. Contours are displayed for U and V from -2.0 to 2.0 and -1.5 to 3.0 with a spacing of 0.2 m/s.

3.2 Example Use Case

To demonstrate the capability of neural networks, we have constructed an example case in which an increasing deterioration of the opening behavior occurs. The neural network can calculate all cases in nearly real-time at once in 0.7 seconds (GPU Quadro M5000). As an example for future use-cases, patient-specific geometry could be determined using clinical imaging methods, and the performance of the heart valve prosthesis could be evaluated by means of deep learning algorithms in real time.

Figure 4: Fluid flow prediction on unseen geometry data with increasing valve malfunction. The velocity in x- and y-direction are color scaled. Contours are displayed for U and V from -2.0 to 2.0 and -1.5 to 3.0 with a spacing of 0.2 m/s.

Both neural networks can predict the flow field through a mechanical heart valve on varying opening angles.

4 Conclusion

We were able to successfully train two neural networks. The results showing that it is feasible to use a neural network to estimate physiological flow fields in the vicinity of prosthetic heart valves (Validation error below 0.06), by only giving geometry data (Image) into the Network. The neural network generates flow field predictions in real-time, which is more than 2500 times faster compared to CFD simulation. Accordingly, there is tremendous potential in the use of AI-based approaches predicting blood flows through heart valves with geometry data as input, in particular in applications where fast fluid mechanic predictions are desired. However, there are also limitations concerning the actual 3D flow, which in this case has been simplified to 2D. The challenge is not the possible extension of the neural network structures to 3D, which is possible by using 3D convolution operations, but the immense computational effort for 3D simulations as training data in supervised deep-learning. Future work will therefore focus on the reduction of training data and the development of unsupervised learning methods based on physical constraints.

Author Statement

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