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REGRESSION OF THE NAVIER-STOKES EQUATION SOLUTIONS FOR PULMONARY AIRWAY FLOW USING NEURAL NETWORKS

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Abstract

Computerized fluid dynamics models of particle deposition in the human airways are used to characterize deposition patterns that enable the study of lung diseases like asthma and chronic obstructive pulmonary disease (COPD). Despite this fact, the influence of patient-specific geometry on the deposition efficiency and patterns is not well documented nor modeled. In part, this is due to the complexity of simulating the full Computational Fluid Dynamics (CFD) solution in patient-specific airway geometries, a factor that becomes a major hurdle for patient-specific studies given the complexity of the geometry of human lungs and their related airflow. In this paper, we present an approximation method based on neural networks to the Navier-Stokes equations that govern airway flow in a Physiologically Realistic Bifurcation (PRB) model for the conducting region of a single generation human airway branch. The flow distribution and deposition of tobacco particles have been simulated for the inspiratory regime using ANSYS Fluent and a neural network has been trained to regress the mean velocity and mass flow components. Our results show that the approximation works well under the modeled assumptions and the serial application of this model to a two-generation airway geometry provides reasonable approximations.

Index Terms—

Particle deposition; neural networks; lung; airways; COPD

1. INTRODUCTION

In recent years, Computational Fluid Dynamics (CFD) has provided insight in the understanding of particle deposition and air flow in human airways, which plays a relevant role in the exploration of diseases like chronic obstructive pulmonary diseases (COPD) and asthma. Current uses of CFD modeling of the human airways are mostly focused on the designing of new aerosol therapies by understanding the deposition regime on canonical human airway geometries. However, the advances on Computed Tomography (CT) have allowed to observe the inter-subject variability and complexity of the airways, which affects the resulting flow [1]. The complexity of the airways and the need for patient-specific results

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for this problem call for the development of models capable of providing an approximation of the numerical solution at a fraction of the computational cost. For this reason, machine learning strategies could constitute a parallel, symbiotic tool for CFD and imaging, potentially helping physicians to identify and diagnose airway lung diseases sooner by means of CFD-inspired biomarkers.

Although many morphometric models have been proposed for a systematic description of the human airways, very few are as concise and realistic as the Physiologically Realistic Bifurcation (PRB) [2] and its successors [3], which while focusing on a single bifurcation can be arranged for the description of a tree. Another popular approach is the use of CT images to reconstruct a 3D model [4], which combined with the recent increase of computational resources and scale simulation models (SRS) has made possible to simulate the turbulent, transient flow in complex lung trees [3, 5]. One disadvantage of this approach is that despite the realism obtained, the geometry cannot be easily parametrized and modified. Therefore, obtaining new geometries and the numerical solution rely on significant time and computational costs. Furthermore, CT-based geometric models are limited by the resolution of the CT scans and reconstructions error introduces errors that may confound the understanding of differences between subjects.

In this work, we propose a semi-automatic method for the creation of a virtual representation of patient-specific human airways based on the 11 parameters of the PRB model, which define an airway bifurcation. We then obtain the numerical solution of the flow using ANSYS Fluent 18.0 for a wide range of cases based on a design of experiments (DOE). Finally, a standard 3-layer fully connected neural network is trained to learn information about the mass flows and velocities at the exit of the branches, that can be used as an input for a new generation of branches. Hence, a relationship between inter-subject geometrical variability and airflow distribution throughout the airways can be exposed and measured.

2. MATERIALS AND METHODS

2.1. Creation of the Geometry

A script based on Python and executed within SpaceClaim has been used to create the geometry using 11 parameters to build each bifurcation as described in the PRB model [2]; namely, the diameters of the parent and daughter branches, their lengths, the branching angles and curvature radii, and the maximum carinal radius. Fig. 1 shows some examples of single bifurcations. By identifying this bifurcation as an *element*, it is possible to concatenate several of them to build more complex structures, including planar and non-planar trees.

2.2. Numerical Simulation

The governing equations of the flow are the continuity and momentum equations from Navier-Stokes, simplified for the incompressible, steady case. A look through the current literature shows that the $k-\omega$ model is widely used for the simulation of flow in human airways [6], [7]. Since the study is not defined for a single Reynolds configuration, the Shear

Stress Transport (SST) model has been employed, as it has proven to work in a wide range of regimes.

Regarding the meshing, due to the enormous number of different geometries, yet similar in aspect, considered and the need for automation, a tetrahedral mesh (refined at the boundary layer region) was used, being the most suitable solution for patient-specific modeling in this problem [8]. A uniform mass-flow condition is set for the cases described, whereas a pressure condition is set at the outlets, which corresponds with the hypothesis of symmetric filling of the lungs. The range of mass flows considered comprises breathing regimes, from resting to exercise activities.

2.3. Machine Learning Regression

Since the goal of this work is to develop a model that correlates the geometry and boundary conditions with the flow distribution, once the geometry has been created as explained in section 2.1, we implemented a regression of the solution via machine learning which provides a specific mathematical model of the problem.

For the training set up, variations of a single bifurcation were created by considering 12 input parameters, given by the 11 geometric parameters of the PRB model plus the mass input flow. In contrast, 7 outputs were considered and measured; namely, the average velocity, average dynamic pressures, and mass flows at both outlets, as well as the wall shear stress (per unit of area). The measurements were integrated from the simulated Navier-Stokes solution as shown in Fig. 2 for each of the input geometries.

The simulated data was selected to consider not only different shapes (focusing on the comparison of input parameters), but also different bifurcation sizes (focusing on the length parameters, globally), particularly useful to get a model able to handle airways belonging to different generations.

Once the data was generated, we employed a machine learning approach to perform the regression through the development of a simple neural network architecture, composed of only three dense layers with 10 neurons in the hidden layer. The network regresses the 7 outputs using an Adam update ($\beta_1=0.9$, $\beta_2=0.999$, $\epsilon=e^{-08}$, decay=0.0) and a loss function customized to optimize both the accuracy and the precision of the prediction. For the accuracy of the method, we consider the mean absolute error over all outputs and the relative error of the mass flows for both outlets given by

$$\mathcal{L}_\mu(y, \hat{y}) = \frac{1}{N} \sum \text{MAE}(y, \hat{y}) + \frac{1}{N} \cdot \lambda \cdot \sum (\text{RE}(y_{mf1}, \hat{y}_{mf1}) - \text{RE}(y_{mf2}, \hat{y}_{mf2})) \quad (1)$$

where MAE indicate the mean absolute error, RE the relative error, y is the true measure, $\hat{y}$ is the predicted measure predicted, and mf1, mf2 represent the mass flows at first and second outlet, respectively. On the other hand, the loss term for the precision, $\mathcal{L}_\sigma$, is computed over 50 replicas of the model inputs to which just small variations (in the range $(-1e-06, 1e-06)$) of the input mass flow are applied. The definition of $\mathcal{L}_\sigma$ is given by:

$$\mathcal{L}_\sigma = \frac{1}{N} \sum_{i=1}^N \left(\sum_{j=1}^M (y_{i,j} - \hat{y}_{i,j})^2 - \left(\frac{1}{M} \sum_{j=1}^M (y_{i,j} - \hat{y}_{i,j}) \right)^2 \right) \quad (2)$$

The idea of the precision term is to make the model more robust to small changes of the entering mass flow and to simulate different mass flows for the daughter branches.

Finally, the total loss function is given by:

$$\mathcal{L}_v(y, \hat{y}) = \mathcal{L}_\mu(y, \hat{y}) + \alpha \cdot \mathcal{L}_\sigma(y, \hat{y}) \quad (3)$$

The best values for λ and α were empirically found by means of grid search cross validation. In this work we used $\lambda = 0.0025$ and $\alpha = 2.5$.

The network was trained on a NVIDIA Titan X GPU machine, using the deep learning framework Keras [9] on top of TensorFlow [10, 11], for 150 epochs at a learning rate of $5e^{-4}$ and batch size of 300.

The network was trained using 2,087 different input solutions. 232 additional input solutions were used for validation to assess model overfitting and performing early stopping of the training process. Tab. 1 shows the ranges for each input parameter that were used to generate the training dataset.

3. RESULTS

3.1. Testing on Single-Branch Model

The proposed neural network method was tested on 774 simulated geometries of a single branch model that were independently generated from the training dataset. The correlation between the regressed solution and the simulated numerical CFD solution for each the seven outputs are presented in Fig. 3. As shown, a very high correlation is obtained for all outputs of both outlets with no apparent bias in the estimation.

3.2. Validation on Two Generations Airway Model

In order to evaluate the potential usability of the proposed method for more complex airway geometries, such as two generations geometries like the one shown in Fig. 5, we created a new dataset of 69 two generation geometries for which we computed the CFD solution for the Navier-Stokes equations. For this case, the single generation neural network was applied in a serial fashion, i.e. we used as input for the entering mass flow of the second bifurcation the two values predicted by the neural network on the outlets of the first generation. The correlations obtained for the mass flows on the two outlets of the two daughter branches in comparison to the numerical simulation of the entire model are shown in Fig. 6. Also, the corresponding Pearson correlation coefficients (with the corresponding p-value) are presented in Tab. 2. Although, as expected, our approximation deteriorates in comparison to the numerical results, the neural network can potentially be used to simulate more complex airway geometries.

4. DISCUSSION

In this work, we have presented a neural network approach for the approximation of the numerical solution to the Navier-Stokes equations for a single generation airway model. The airway generation model was based on the PRB model, and its parameters were chosen based on data obtained from CT images to match the human anatomy scale.

The results obtained using the neural network show that the proposed approach is appropriate for simulating the mass flows and output velocities in human airways. The validation on the two generation geometries indicates that despite the simplicity of the model, just a few adjustments may potentially make it a good candidate for the regression of the complex numerical solution of the turbulent flow and particle deposition in airways, which is currently being complemented hand by hand with experimental validation [12].

The assessment of a well-adjusted double bifurcation algorithm would constitute a big leap as it could be easily extended for a greater number of generations up to the conducting airways. To this end, the neural network should be trained with single branches where the mass flows enter with different angles and orientations to help the network better predict the output mass flows regardless of the input. Also, alternative approaches to take into account for the regression of the numerical solution in multiple generation airway geometries could be the use of recurrent neural architectures, such as the LSTM architecture [13], that will fully model the serial nature of the solution. Finally, the presented model is a proof of concept that needs to be tested and validated in full airway trees. We believe this presented work warrants further work in this direction.

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Fig. 1.
Examples of the variations of a single bifurcation generated.

Fig. 2.

Velocity contours obtained via simulation at the plane of symmetry, inlet and outlets

Fig. 3.

Correlation obtained in comparison to the numerical solution of 774 testing points simulating a single branch airway for mean velocity (top), mass flow (middle), and dynamic pressure (bottom). The first column show results on the first outlet, while the second presents the correlation for the second outlet. Pearson correlation coefficient is shown on each figure.

Fig. 4.
Correlation between our method and the numerical CFD solution for wall shear stress (same for both outlets).

Fig. 5.

Example of a two-generations geometry used for validation. Dau stands for daughter, while Out is used to indicate an outlet.

Fig. 6.

Correlation obtained when simulating a two generations airway model by using the predicted mass flow on the first branch as input for the two daughter branches. First row shows the mass flow correlation on the two outlets of the first daughter (dauA), while on the second row the mass flow correlation of both outlets for the second daughter branch (dauB) is presented.

Table 1.

Ranges of input parameters used for training. g1 to g11 represents the geometric parameters of the PRB model and mf_i is the mass input flow.

	g1	g2	g3	g4	g5	g6
min	3.0	4.0	1.9	3.0	1.9	3.0
max	4.6	14.0	3.0	14.0	3.0	11.0
	g7	g8	g9	g10	g11	mf_i
min	28.0	28.0	14.0	15.2	0.19	$1.02e^{-5}$
max	55.0	52.0	14.0	30.0	0.45	$1.24e^{-4}$

Table 2.

Pearson correlation coefficients (ρ) and the corresponding p-values obtained for the mass flows at the two outlets of the two daughter branches.

	ρ	p-value
Daughter A Outlet 1	0.75	$p < 0.001$
Daughter A Outlet 2	0.67	$p < 0.001$
Daughter B Outlet 1	0.70	$p < 0.001$
Daughter B Outlet 2	0.80	$p < 0.001$