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Numerical Simulation of the Human Lung: A Two-scale Approach

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Abstract

In this paper we introduce a two-scale model for the numerical simulation of the human lung. The airflow in the upper, resolvable part of the human lungs is modelled by the Navier-Stokes equations, which couple to a dyadic bronchiole tree model through boundary conditions. This model depends mainly on the generation, where the inlet is located, and the radius of the bronchiole at this generation. In the bronchioles a linear flow is assumed, hence the Hagen-Poiseuille formula can be applied. The pressure at the alveoles and the starting resistance for the dyadic tree are used as input parameters. To illustrate the approach, we simulate a patient-specific human lung geometry with a Lattice-Boltzmann method and show qualitative convergence results for the pressure drop as well as a comparison with Neumann boundary conditions that are commonly used in one-scale models. Results for an overall flux of $Q = 150 \text{ ml/s}$, which corresponds to a Reynolds number of $Re \approx 1650$, are presented.

1 Introduction

The numerical simulation of the full human respiratory system corresponds to one of the *Grand Challenges* in scientific computing nowadays. The field of applications related to this capability is tremendous and encompasses e.g. the analysis beforehand of possible implications on the respiratory tract due to surgery and the environmental impact on lung. The main difficulties are not only related to the complex geometry but also to a highly complex multiphysics phenomenology involving multi-scale features.

Our goal in this paper is to present a feasibility study related to a newly developed numerical scheme allowing to compute specifically the flow behaviour in the respiratory tract. The proposed approach is based on the coupling of a bronchiole model with a macroscopic 3D Navier-Stokes model. Similar results are proposed and discussed in other papers as well (e.g. [5] and references therein) but with a different modelling approach and usually with a much smaller Reynolds number $Re \approx 800$. In this paper we consider this coupling in a pseudo-stationary set up. The considered bronchiole model allows to represent the smaller scales of the bronchioles that can not be resolved using standard medical imaging like computer tomography (CT) or Magnetic Resonance Imaging (MRI). The proposed coupled approach shows good results in terms of stability and convergence.

The paper is organized as follows: In Section 2, we describe the proposed two-scale model and depict the model coupling by means of adequate Dirichlet boundary conditions. Numerical results calculated for a patient-specific lung geometry are presented in Section 3. This section emphasizes both the practical usability of the proposed scheme as well as the ability to use it in the context of high performance computing (HPC). The simulation results obtained with this new model are discussed and compared to those achieved with standard boundary conditions.

2 Two-scale Model

The essential point of the two-scale model is the coupling of the model for the upper, resolvable lung geometry, which is made up of the trachea and the bronchi, to the model for the lower part of the lungs, the bronchioles. At the outlets of the bronchi, we take a bronchiole tree model of the lower respiratory system into account. This model yields an inflow condition at each outlet depending mainly on the generation and the area of each outlet as well as the pressure in the alveoles and the resistances due to the radius of the bronchioles as illustrated in Figure 1.

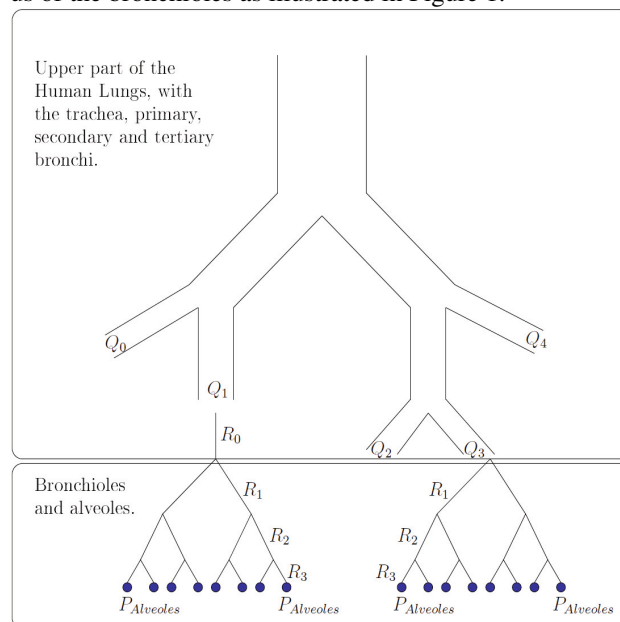


Figure 1 Scheme of the coupling between the model for the upper geometry and the lower lung model.

2.1 Bronchiole Model

Our main requirement for the model used for the lower hu-

man lungs is to provide adequate boundary conditions for simulations of the upper part of the lungs. For fluid flow simulations this means that we have to extract a flow profile that reflects the complete flux in the lower lungs. In order to achieve this, we assume the airflow in the bronchioles to be linear, which means Poiseuille's law is satisfied. To keep the model as simple as possible, we think of a dyadic tree representing the bronchioles and assume equal resistances for all bronchioles of the same Weibel generation [10]. Also, the resistances decrease uniformly by a factor $\alpha \approx 1.63$, which results in $R_i = R_0 \alpha^i$ for the resistances R_i of the i -th generation. This is reasonable due to the fact that the radius and length of each bronchiole is decreasing uniformly. We assume further that the pressure is the same for each alveolus [4].

The formula of Hagen-Poiseuille combined with a parabolic flow profile leads to a relation between the flow Q and the maximum velocity v_{max} of the flow profile on each outlet of the upper airways.

If we substitute the parabolic flow profile

$$v_{max} = \frac{\Delta p}{4\mu l} r^2 \quad (1)$$

into the formula of Hagen-Poiseuille

$$Q = \frac{8\mu l \Delta p}{\pi r^4} \quad (2)$$

with Δp the pressure drop,
 l the length of pipe,
 μ the dynamic viscosity,
 Q the volumetric flow rate,
 r the radius,

we get the relation

$$v_{max} = \frac{2}{\pi r^2} Q \quad (3)$$

between the flow and the maximum velocity in the parabolic flow profile. We can modify this to the more general case that uses the surface A (which can be expressed in terms of number of voxels) of the outlet:

$$v_{max} = \frac{2}{A} Q. \quad (4)$$

However we still assume a circular outlet, as this is a precondition for the parabolic flow profile as well as the formula of Hagen-Poiseuille.

Q will be determined through the tree model using the electric analogy $U=RI$. U corresponds to the pressure difference Δp , R is the resistance and I the flux Q .

We can consider the dyadic tree to be a series of resistances, the first one serial to the next ones, which are parallel to each other and so on. Hence, for the resistances we get

$$R = R_j + \left(\frac{2}{R_{j+1}}\right)^{-1} + \left(\frac{4}{R_{j+2}}\right)^{-1} + \dots + \left(\frac{2^k}{R_k}\right)^{-1}, \quad k > j, \quad (5)$$

with $k = \#(\text{generations}) - \#(\text{generations of the upper connected tree})$, which yields

$$R = \sum_{i=j}^k \left(\frac{2^i}{R_i}\right)^{-1}, \quad (6)$$

where j denotes the generation number, at which the tree model is attached to the upper geometry (see Figure 1).

Due to the assumption of equal resistances per generation, the pressure in the alveoles (level K) corresponds to the pressure at the outlets (level k) of the upper geometry

$$P_K = P_{K-1} = \dots = P_k, \quad K > k. \quad (7)$$

Putting the equations above together, we obtain

$$Q = \frac{P}{R_{total}} = \frac{P_k}{\sum_{i=j}^k \left(\frac{2^i}{R_i}\right)^{-1}} = \frac{P_k}{\sum_{i=j}^k \frac{R_i}{2^i}}. \quad (8)$$

As the generation number k , where this flow condition couples with the upper tree, as well as the area A is given, we have two parameters left that have to be set. The former being the pressure $P_k = P_{Alveoles}$, the latter being the initial resistance R_0 of the largest bronchiole. Both can be distinguished roughly by literature values, but have to be fine-tuned in order to match with volume flow measurements from a respiration cycle.

2.2 Model for the Upper Lungs

The fluid flow in the resolvable part up to the 9th generation [10] of the human lungs is described with the incompressible Navier-Stokes equations [2]. This is justifiable due to the low Mach number regime and the Newtonian characteristics of air. The model is completed by Dirichlet boundary conditions at the lower inflows, which are defined according to (4), and with Neumann boundary conditions at the upper outlet (see Figure 1).

3 Numerical Experiments

3.1 Case Study

As test case, we consider the lung of a middle-aged male human. The computational domain was extracted from CT data with a resolution of 0.4mm.

In order to set up flow simulations, it is necessary to determine a couple of parameters. These are primarily the overall flux and the maximum flux. Having those two values determined, one can easily calculate the corresponding velocity profiles (see Figure 2) and therefore the Reynolds number taking the maximum diameter at the trachea as characteristic length and the kinematic viscosity of the system into account.

Assuming a sinusoidal profile for the inhalation and taking the overall flux of $Q = 150ml/s$ for a sitting awake male person, measured by the International Commission on Radiological Protection (ICRP), we get a maximum flux of $Q_{max} = 236ml/s$ that can be calculated using the tidal volume $V_t = 0.75l$ per period and the respiration frequency $f_R = 12min^{-1}$. Half a period is assumed to take $T = 2.5s$

and hence the inhaled air is $V_{t/2} = 0.75/2 l$ [9].

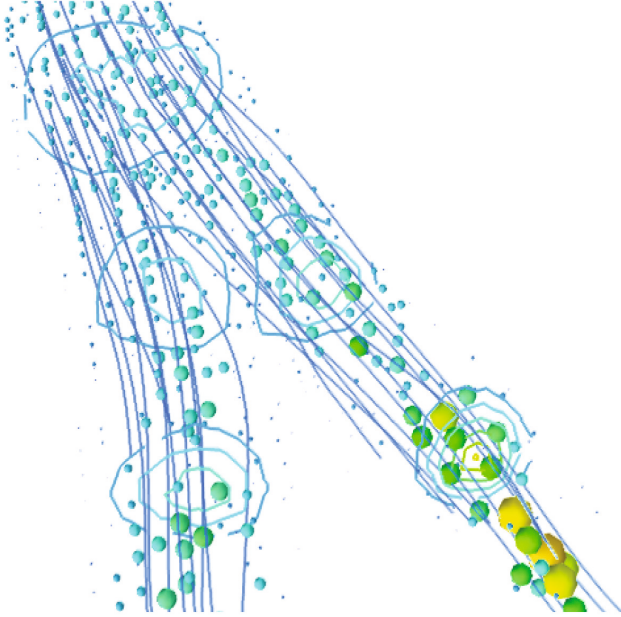


Figure 2 Contours, spheres and streamlines of the velocity distribution on two inlets at Weibel generation 7, resp. 8.

3.2 Simulation Details

To simulate the desired mean flow of $Q = 150 ml/s$, which corresponds to an everyday situation, we get a Reynolds number of $Re \approx 1650$. To solve the incompressible Navier-Stokes equations we use a $D3Q19$ Lattice-Boltzmann model with BGK collision operator. This discretization approach requires the computational domain to be a uniform, hence, a voxel mesh [1]. The patient specific mesh that was created in a preprocessing step [3] consists of approximately 2.33 million fluid voxels, which results in about 44.3 million unknowns for the $D3Q19$ scheme. However to get stable results, we need to refine the mesh, which yields over 354 million unknowns. Yet for more evidence about stability, we need to compare different geometry set ups.

The simulations were done on the HC3 supercomputer at the KIT [8] with 90 cores on a level 2 refined voxel mesh. For 250.000 time-steps the computation took 12 hours. We used the OpenLB [6,7] Open Source software package for our computations.

3.3 Convergence of Pressure Drop

The pressure drop between each inflow and the trachea is a very good indicator to see if the (stationary) simulation converges to a steady state. In an ideal scenario, the pressure drop rises from zero to some positive value, while raising the inflow velocity, and stays constant over time when the velocity profile does not change any longer.

We let the velocity increase linearly from zero to the desired maximum value over 100.000 discrete time-steps and keep it constant from there onwards. However as soon as the velocity reaches its maximum, acoustic waves that re-

flect on the trachea inlet run through the system and result in an oscillation of the pressure. These acoustic waves occur due to the so called “do-nothing” boundary conditions that are used at the trachea inlet.

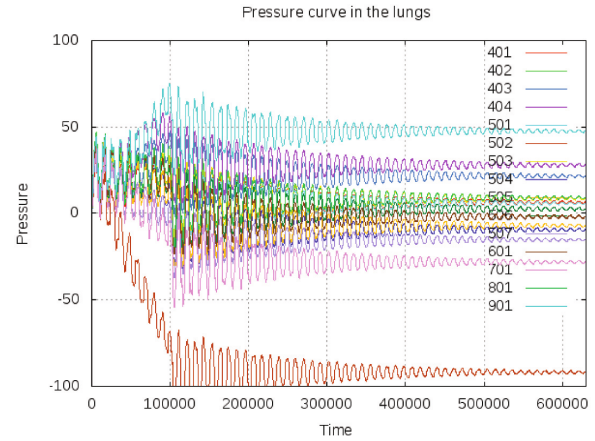


Figure 3 Plot of the pressure drop between the different inflows at the bronchioles and the trachea inlet. Oscillations exist due to an acoustic wave that is reflected (“do-nothing” boundary condition) at the trachea outlet. Velocity was increased linearly from 0 to the maximum value at each bronchiole inflow over 100,000 discrete time-steps. The captions on the right hand side are sorted by the Weibel generation number, which is the first digit, and afterwards enumerated in no special order.

The negative value on inlet 502 exists due to a Venturi effect that can nicely be validated having a look at the geometry (Figure 4).

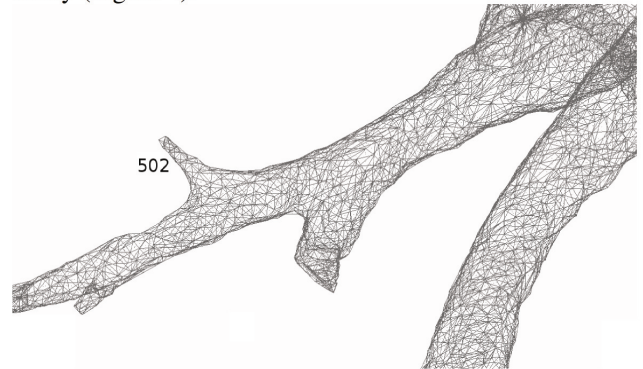


Figure 4 Geometry of the Human Lungs. On inlet 502 exists a Venturi effect due to small inlet 502 and the relatively large flow in the “main” bronchiole. This results in the negative pressure at this inlet.

3.4 Flow profile

Reconsidering the main prospect of the proposed model, which was to create physically reasonable boundary conditions for the human lungs, it can be seen in Figure 5 that the expected Poiseuille profile develops in the trachea. To present detailed studies, different patient-specific geometries have to be evaluated. However Figure 5 validates the model qualitatively.

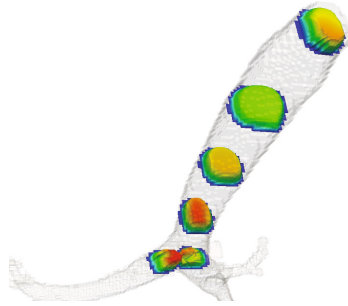


Figure 5 Poiseuille profile that develops in the trachea. The bad resolution of the data is due to visualizing restrictions. Only every 4th point was stored because of the massive load of data (about 354 million of unknowns).

3.5 Comparison of Different Boundary Conditions

It is easy to see that due to the so-called “do-nothing” boundary conditions at the outlets of the lungs the flow is very unequally distributed and takes the shortest way possible through the tree (see Figure 6). This effect is accounted for by the non-physically cut of the geometry, which is necessary due to the bad resolution of the CT scans. With the tree model (see Figure 7) we take care of exactly this flaw in the geometry. Also we get a much better convergence with respect to the pressure drop and the results are more stable for high Reynolds numbers.

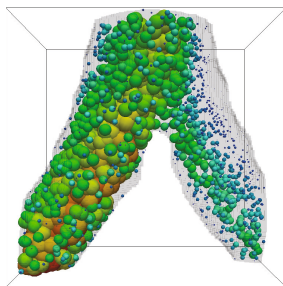


Figure 6 First bifurcation simulated with “do-nothing” boundary conditions.

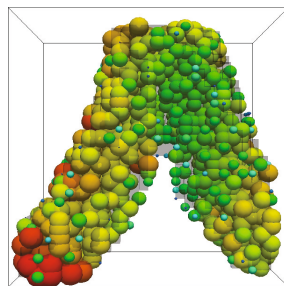


Figure 7 First bifurcation simulated with boundary conditions from the tree model.

4 Conclusions

We have introduced a new model for the boundary conditions at the lower bronchiole inlets of the human lungs and coupled this model with a 3D Navier-Stokes solver successfully. It was shown that the proposed method is efficient, that a physically reasonable flow profile develops and that patient specific simulations converge with respect to the pressure drop in the lungs. A comparison between the conventional boundary conditions and the new, more specific, boundary conditions clearly showed good results in terms of stability and convergence. The upcoming steps will include parameter studies that re-

flect pathological lungs, e.g. asthma, and fluxes for heavy exercise, to analyse the resulting flow profile. Also the model will be enhanced towards simulations of instationary flow. The comparison of the obtained numerical results with medically measured data will be subject of the forthcoming paper.

5 Acknowledgements

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