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NUMERICALLY PREDICTED FLOW IN CENTRAL AIRWAYS: MODELLING, SIMULATION AND INITIAL ANALYSIS

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ABSTRACT

To analyse the dynamic flow in central airways, a workflow has been established which finally enables numerical simulation with simultaneous consideration of natural deformed geometries and inversion of flow direction. Besides a comprehensive description of the interdisciplinary methods, variations of boundary conditions and parameters are discussed, as well as method validations are presented. Finally, selected insights to the flow field reveal important features and emphasise the necessity of dynamic simulations.

INTRODUCTION AND OBJECTIVES

In case of an acute lung injury artifical ventilation is the only known life-sustaining therapy. Unfortunately, the parameters used for the ventilation are primarily based on empirical models, but not on understanding of physiology and physical phenomena. Therefore artificial ventilation is often accompanied by serious side effects and a high mortality of the patient. To ameliorate this situation, several interdisciplinary projects funded by the German Research Foundation (DFG) have been launched in order to provide deepened understanding of the fluid and structural physics present in natural geometries of the airways. In this framework the cooperation amongst medical and engineering scientists allows to judge different ventilation strategies and provides the potential to develop new protective ventilation strategies, or at least a set of parameters based on observed physics.

As a starting point, the aim of the present work is to predict the flow physics, up to this point unknown, and to describe quantitatively the functional relevance of temporary and fixed deformations in the central airways. Therefore, numerical simulation of the unsteady flow in the upper airways have to be enabled, performed and analysed. The unsteady investigations have to account at least for dynamic geometry changes and the oscillatory flow, whereas initial simulations of the steady base flow determine important parameters and provide first insights to the flow regime.

The description of the interdisciplinary methodology, which results in a workflow to enable dynamic simulations is given at first. Subsequently, the numerical methods, parameters and configurations investigated are summarised, before the method validation and parameter variations are briefly discussed. The initial analysis of steady, unsteady and dynamic simulations complements the work presented.

INTERDISCIPLINARY WORKFLOW

Medical relevance and natural reference of the numerical investigations will be achieved by the interdisciplinary work of specialists in radiology, medical informatics and fluid mechanics. Especially, the acquisition of dynamic, human or animal airway geometries, their preparation and realistic boundary conditions require the abilities and methodic features of non-engineering partners. In order to investigate the flow in several different, mainly natural geometries and to extract the differences and functional relevance due to geometry changes, an automated workflow has been developed. A general overview of the multi-directional linked work packages is given in figure 1.

For gathering dynamic geometries of the central airways, either human or animal, the radiologic imaging method Four-Dimensional Computed Tomography (4D-CT) has been employed. The four-dimensional (spatial and temporal) output contains several stacks of two-dimensional gray value images over time, in which each stack build up a

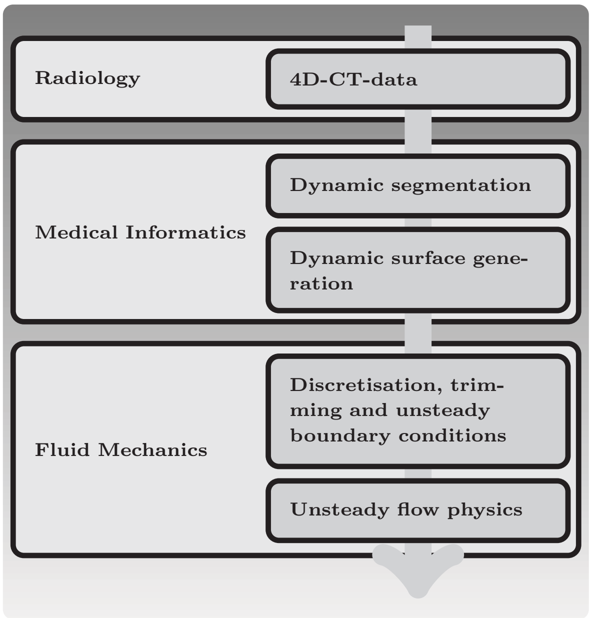

Figure 1: Interdisciplinarity and realised workflow.

volume. By means of image segmentation anatomical structures such as the bronchial tree can be extracted from the images (cf. figure 2). A time-resolved surface representation can be generated by processing the temporal stacks. Therefore extended adaptive region growing (Wolber et al., 2008) is utilised to segment the anatomic volume with as many bifurcation levels per timestep as possible. Dependant on the image quality and due to the partial volume effect, the current method achieves up to 7 levels, whereas the optical inspection allows more levels. In the future, with the aid of Bayesian Tracking (Schaap et al., 2007) algorithmically irrecognisable tubular structures can be found based on likelihood estimations allowing to bridge stenosis.

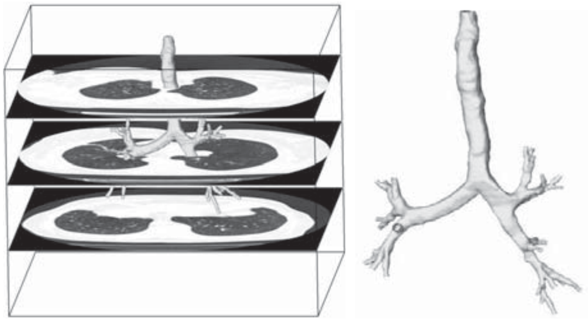

Figure 2: Exemplary CT images and cut surface of a human bronchial tree prepared for flow simulation.

The bronchial surface (figure 2) is generated from the segmented voxels by smoothing, refinement and magnification, which is necessary to represent the anatomy realistically. To prescribe the surface deformation for the simulation, displacement fields are extracted between successive temporal surface representations. The skeleton of the surface is finally used to trim the surface axis-normal such that planar end-faces for numerical boundary conditions limit the fluid domain. Given by the image modalities, a high temporal resolution leads to a lower resolution in space. Thus, a tradeoff between temporal and spatial resolution has to be made. The temporal resolution required for simulation is achieved by interpolation (e.g. linear) between displacements fields in succession. The dynamic geometries and extracted boundary conditions are then used for numerical flow investigations over the whole breathing cycle.

NUMERICAL METHODS AND PARAMETERS

For flow simulation two different numerical approaches are considered.

The prediction of the steady base flow with respect to parameter variations has been performed using the commercial package StarCD, a general purpose CFD application using the Finite-Volume method (CD-adapco, 2005). This code is capable of solving steady-state or transient problems, compressible or incompressible, and under laminar and turbulent flow regimes using standard two-equation turbulence models. The velocity-pressure coupling is accomplished here using a SIMPLE algorithm. The convection scheme used was StarCD's proprietary "Monotone Advection and Reconstruction Scheme" (MARS), a second-order accurate scheme with multi-dimensional TVD algorithm. The volume inside the airway geometry has been discretised with an unstructured mesh based on tetrahedrons (figure 3 left).

For flow simulations in dynamically changing geometries the numerical method employed must incorporate any kind of adaption for the spatial discretisation or domain. A method developed for problems with natural geometries is the Immersed Boundary method (IB) originally proposed by Peskin (1972). In order to avoid grid deformation algorithms, which are not suited for large deformations, and also timestep-wise regeneration of the grid requiring interpolation of field quantities, the IB method is preferred. This method together with a proper computational infrastructure has been implemented in a variant of the in-house flow solver ELAN at TU Berlin (Hylla, 2008). The original code by Xue (1998) based on the Finite-Volume method and general curvilinear coordinates has been reduced to unstructured Cartesian meshes with local refinement (figure 3 right), which allows to use the advantages of the IB method to full capacity.

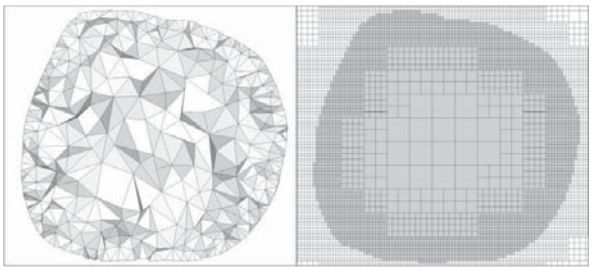

Figure 3: Representative grid slices with tetrahedrons (left) and Cartesian hexahedrons (right).

In each timestep the identification and marking of the computational domain w.r.t. the actual geometry shape is performed to distinguish between fluid and non-fluid regions (fluid region indicated by grey colour in figure 3 right). The treatment of the immersed boundaries originates from the "ghost-cell" approach, whereas fluxes and gradients are corrected directly without storing any value in ghost-cells. The further numerical methods utilised in the code are a SIMPLE pressure correction algorithm, upwind and central difference schemes for convection with flux blending and a BiCG-stabilised solver. The code, permanently under development, does not yet allow for turbulence models in combination with the IB method, but as examined in steady investigations initial turbulence decays shortly, and thus turbulence modelling is not required.

In the simulations performed air under standard conditions has been considered as fluid. For the parameter investigations in a steady geometry the volume fluxes 125, 243 and 333 ml/s and three different shaped profiles (block, laminar, double-peak) have been applied to the inlet boundary. The outlet boundaries require any reasonable model for flux or pressure, because very few is known here in advance, and measurements are hardly possible. The simplest approach used is the explicit distribution of the flux fraction proportional to the fraction of the total outlet area (referred to as *tree model*). The local volume flux at the numerous outlets can be determined more realistically with an additional lung-shaped volume and specified pressure on the envelope (*lung model*). For the simulations with changing flow direction the volume flux is prescribed by a sinusoidal curve (with the average flux matching the steady ones given above) and applied to the "inlets" and "outlets" respectively. In the future the boundary models will be extended in order to account for the lung impedances.

CONFIGURATIONS INVESTIGATED

The parameter variations have been conducted in a single surface representation taken from maximum inspiratory condition of human airways (already shown in figure 2). The Reynolds number based on the diameter of the trachea, kinematic viscosity and mean velocities prescribed by the volume flux, takes the values 1 185, 2 300 and 3 155. The spatial discretisation of the fluid region involves 730 000 tetrahedrons or 6 200 000 hexahedrons, respectively. The comparably higher resolution of the grid for the IB method is due to the appropriate resolution of the small tubes at high bifurcation levels, which has not been considered for the tetrahedral grid. In order to analyse the influence of the dynamically changing surface, the oscillatory flow has been simulated in steady and generically deformed geometry of the human airways.

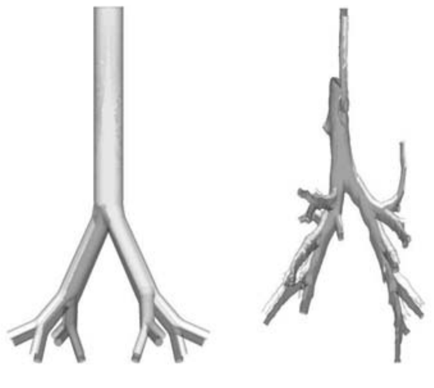

Figure 4: Weibel lung model (left) and porcine bronchial tree (right) with their maximal deformed geometry shapes.

The Immersed Boundary code has been tested inter alia on a generic lung geometry, which was specified by Weibel (1963) as lung model A (figure 4 left). This model consists of four branch generations assembled by joined pipes with different diameters and 60° branching angles. Steady simulations were carried out for increasing Reynolds numbers between 10 and 2 000 with a fluid region spatially resolved by 352 000 cells (Hylla et al., 2009). Furthermore, unsteady and dynamic simulations with generic deformation and sinusoidal changing volume flux has been performed at Reynolds number 2 000 on a refined grid with on average 503 000 cells in the fluid region.

A well resolved dynamic geometry has been acquired via CT from artificially ventilated porcine airways (figure 4 right), which are known to be very similar to human airways. The natural deformations between 10 surfaces representing a single respiration cycle were initially extracted employing a rigid registration with subsequent point-to-point mapping. The investigation of the dynamic flow behaviour has been started recently with approximately 500 000 spatial cells in the first instance.

METHOD VALIDATION

The implementation of the IB method has been validated using testcases of varying complexity, including the Weibel lung model. The results of the validation w.r.t. steady simulations published in Hylla et al. (2009) reveal a very good agreement for the Weibel lung with numerical experiments by Kabilan et al. (2007). Furthermore, the results obtained in the steady human lung have been compared between the commercial StarCD and the in-house IB code. The results shown in figure 5 demonstrate acceptable results, whereas the differences are attributed to the considerably higher resolution in the IB mesh, as well as to slightly different numerics and outflow boundary conditions. The combination of Immersed Boundary and the flux-based Finite-Volume method is the basis for flow quantities and fluxes following the segmented surface, although the spatial discretisation resembles a stepwise approximation (cf. figure 3 right).

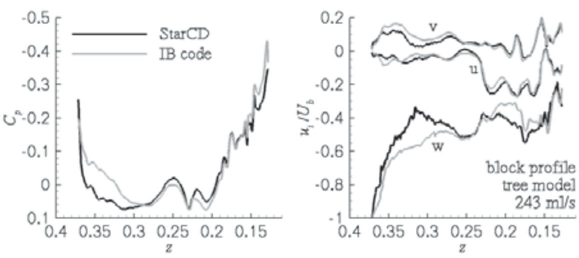

Figure 5: Pressure coefficient C_p (left) and normalised velocity components u_i/U_b (right) in a volume line (cf. figure 6) compared between StarCD and IB code.

PRELIMINARY INVESTIGATIONS

The simulations of the steady base flow have been initialised in a first step with turbulent content in the field and on the inlet boundary. The turbulent kinetic energy reaches near zero levels very shortly behind the inlet, thus a laminar state is achieved and no high-grade turbulence modelling is necessary. This has been observed for all Reynolds numbers (up to 3 155) being investigated.

The variations in volume flux, inlet profile and flux distribution on the outlet confirm that realistic boundary conditions are important. A summary of the obtained results is shown in figure 6 using the pressure coefficient C_p and the vertical velocity component w along a volume line, whereas a single parameter is varied and the two others are fixed. The variation of the volume flux has neglectable influence to the normalised velocity field, but as typical for such flows the pressure drop in the lower airways increases with amplified flux. Moderate influence could be observed for different inlet profiles. The comparably large differences for the laminar profile reflect the doubled velocity magnitude compared

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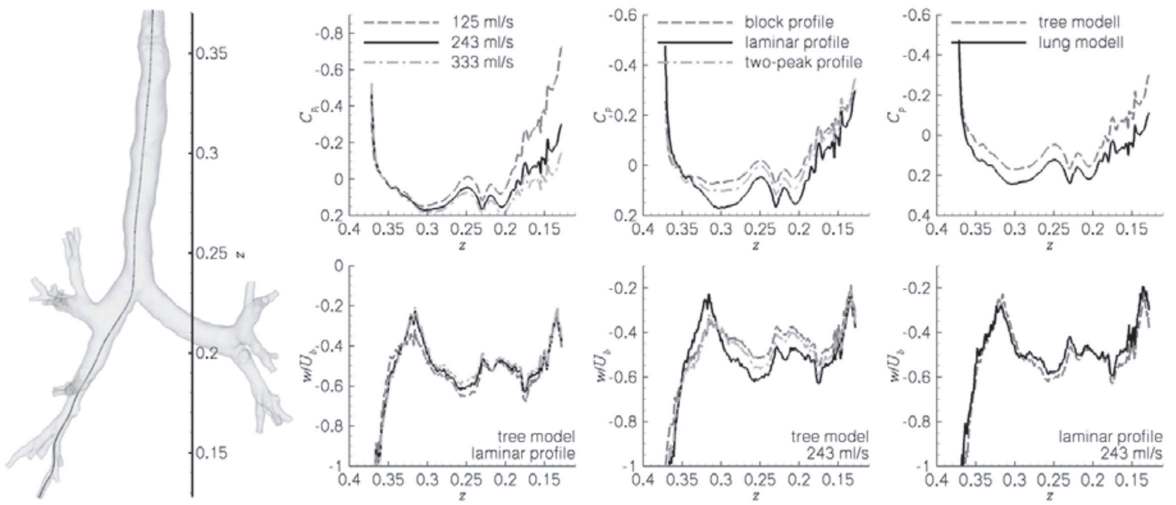

Figure 6: Pressure coefficient C_p and normalised vertical velocity w/U_b in a volume line (sketch) with variation of volume flux (left), inlet profile (middle) and outlet flux distribution (right).

to the block profile in the bronchus centre.

The simple tree model with outlet fluxes proportional to the area fraction implies a strong constraint to the velocity field, because the velocity magnitude for each outflow is identic and fixed. The application of a more realistic boundary condition, which allows regulation of the local volume flux w.r.t. the pressure, leads to maximum differences of $\pm 40\%$ in particular fractions compared to the area-based distribution. As a result the pressure load is increased globally (cf. figure 6 right).

For the further investigations the volume flux used is 243 ml/s, which is appropriate for tidal breathing. A calibration of the volume flux for the separated outflow boundaries (or in the case of expiration the separated inflow boundaries) is applied, which takes into account the neglected lower airways particularly. Due to the lack of further upstream geometry, e.g. larynx and nose, the laminar inlet profile is preferred, which is appropriate for laminar pipe flow.

INITIAL FLOW ANALYSIS

The understanding of the flow can be enhanced firstly by evaluating the steady flow field. Due to varying bifurcation angles, the predicted velocity field comprise diverse areas. On the one hand there are core regions with relatively high velocity, and on the other hand there are bypass-like regions. This is demonstrated by the local velocity field shown in figure 7 using magnitude and planar profiles at different positions.

Figure 7: Velocity magnitude (left) and planar velocity profiles (right) in axis-normal slices of the human lung geometry.

Independent of the configuration investigated, the steady simulations predict counter-rotating vortex rolls throughout all branch levels (figure 8), whose effect can be interpreted as a natural "wash-out" of the airways. In the context of an obstructive pulmonary disease the hypothesis remains to be proven, that any disturbance of these vortical structures affects the self-purification of the central airways, and therefore is an important component for possible obstructions.

Another issue often addressed in flow analysis of airways is the occurrence of separation regions close behind bifurcations. Quite often such findings are based on two-dimensional investigations, for example by Wilquem and Degrez (1997). In the steady simulations performed within the human and in the Weibel lung no separation w.r.t. the flow direction could be observed. Nevertheless there is obviously separation of the in-plane secondary flow, which is the result or cause of the aforementioned helical vortices.

UNSTEADY AND DYNAMIC SIMULATIONS

The unsteady flow with changing flow direction has been investigated successfully in the steady Weibel and human lung. The respiration cycle modelled by sinusoidally changing volume flux varies within arbitrary chosen but reasonable time periods of 4.0s for both, resolved with 160 and 120 timesteps respectively. The exemplary results depicted for the human lung in figure 9 allow to detect velocity profiles with a double-peak shape (projected to a plane), which have been found previously in experiment by Riethmuller (2000). These unsteady profiles differ significantly from the results of the steady regime, which emphasises the importance of nonstationary investigations. The double-peak shape found experimentally originates the application of a similar inlet velocity profile, constructed by polynomials, in order to force such profiles in the flow field also for the steady case, but with moderate success.

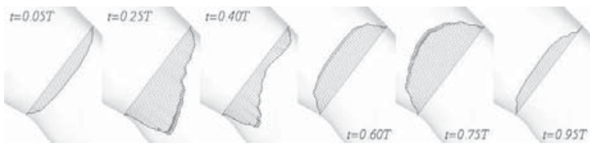

Figure 9: Velocity profiles in a central plane behind the first bifurcation of the human lung geometry for several stages in an oscillatory flow.

At higher bifurcation levels, the double-peak profiles are also visible during expiration. Their shape results in the

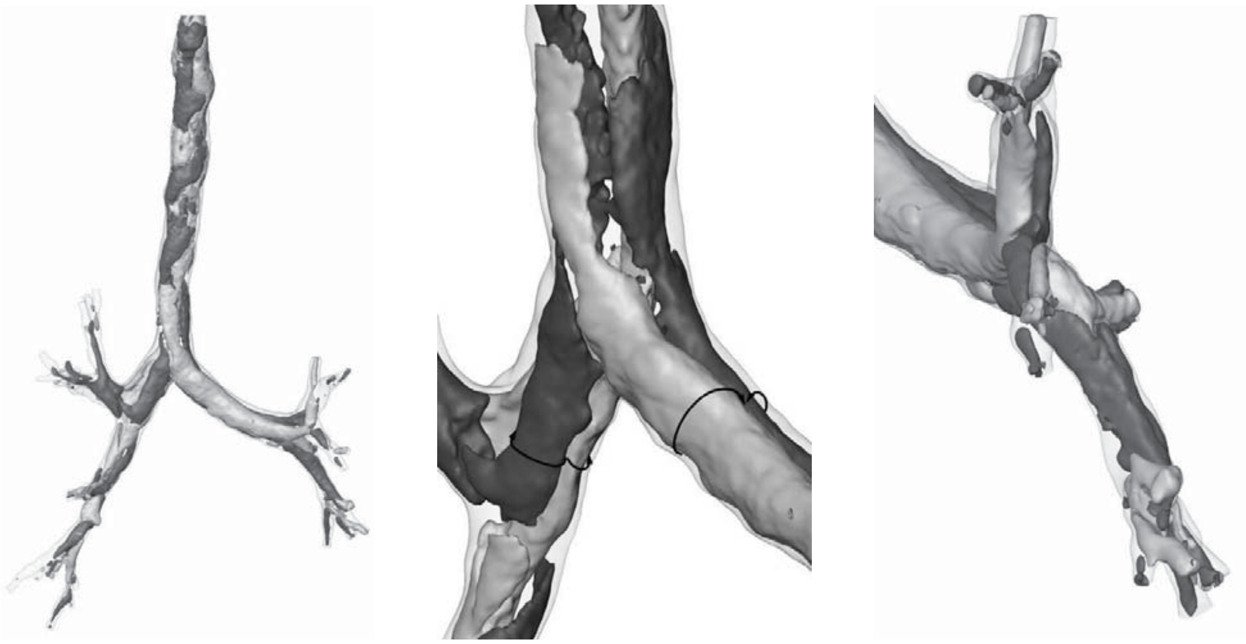

Figure 8: Counter-rotating vortex rolls represented by isosurfaces of positive (dark) and negative (light) helicity: overview (left), at first bifurcation (middle), at further bifurcations (right).

higher momentum of the velocity core region, whose inertia is responsible for the delay in changing the fluid's local direction. The continuous change of the flow direction increases the mixture of the fluid inside the vessels, thus the above mentioned bypass character of some regions is slightly reduced compared to the steady field. However, as already found in the steady results, the unsteady flow field predicted in the human lung reveals the absence of noticeable separation w.r.t. the flow direction throughout the whole respiration cycle.

A further increase in complexity has been introduced by the simulation of the oscillatory flow in the sinusoidal changing human lung with constant generic deformations towards the surface normals. In comparison to the flow in steady geometry, the velocity profiles predicted are slightly flattened under expiration, whereas the peaks are strengthened in inspiration (cf. figure 10). Taking into account the perfect phase agreement of flow reversal and the small deformations applied, it is self-evident that possible phase shifts or larger deformations will intensify the differences.

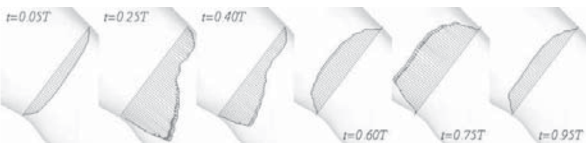

Figure 10: Velocity profiles in a central plane behind the first bifurcation of the dynamically deformed human lung geometry for several stages in an oscillatory flow.

In figure 11 the velocity profiles of simulations with oscillatory direction are compared between steady geometry and dynamically deformed geometry in the Weibel lung. In order to recognise the portion of the deformation velocity included in the absolute profile, the velocity relative to the geometry is additionally shown for the dynamic case. The position of the profiles depicted is located in the middle of the pipe with the second largest diameter, and hence represents pipe flow character for the steady geometry. As the difference of the profiles is a result of the surface deformation the necessity of dynamic simulations is shown. This becomes more evident considering that the applied generic deformation mimics the global behaviour of central airways. Although the influence of special details like the lung impedances are currently not known, it can be safely assumed that the geometry deformation strongly affects the velocity field and must therefore be considered for reliable flow predictions in central airways.

The counter-rotating vortices observed in the steady investigations are also present in the unsteady and dynamic case. Although the local helicity magnitude changes primarily sinusoidal, the rotational direction of the main structures is conserved, which is consistent with the principle of angular momentum conservation in fluid mechanics. However, in the steady case and under inspiratory condition in the unsteady case, the vortex rolls emerge in each branch directly after flow partitioning at bifurcations. In the expiratory phase, a pair of helical regions also emerge in each branch, but has to merge with other pairs at the bifurcations. Thus, in general more than a single pair of distinct positive and negative helicity regions is present behind the branch fusions (cf. figure 12), depending on the number of bifurcations nearby. The merging or suppression of helical regions evolves in a very narrow region, and therefore several pairs can only be observed in the vicinity of bifurcations.

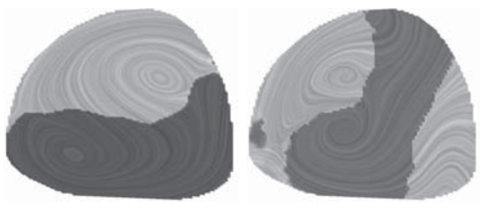

Figure 12: Line-integral-convolution and regions of positive (dark) and negative (light) helicity in an axis-normal slice close before second bifurcation of the human lung: extremal inspiratory (left) and expiratory condition (right).

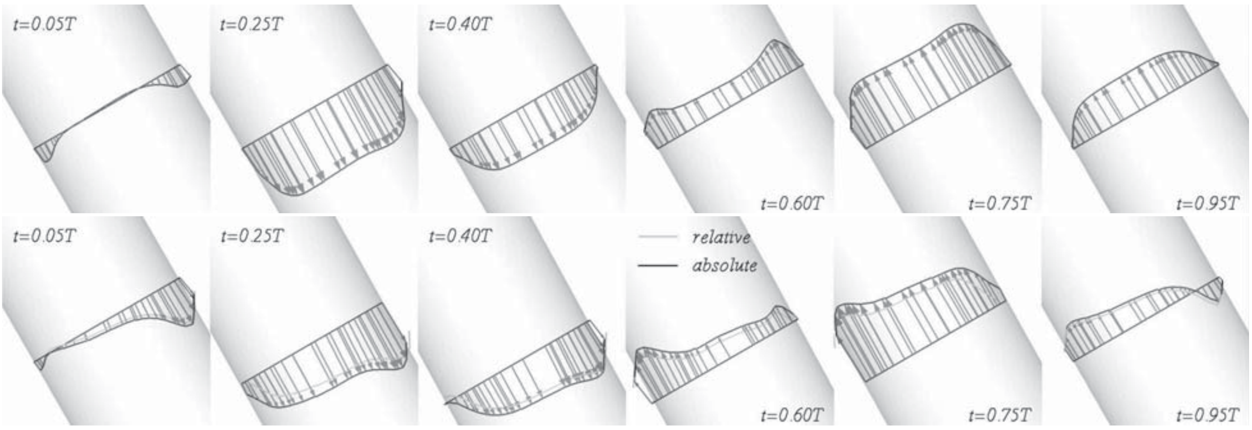

Figure 11: Velocity profiles in a central plane at half second branch of the Weibel lung for several stages in an oscillatory flow (top) and dynamically deformed geometry in addition (bottom).

CONCLUSIONS AND OUTLOOK

For investigations of the unsteady oscillatory flow in central airways a workflow has been developed and established. Based on the interdisciplinary work of different departments, this workflow allows to extract geometries representing the natural anatomy of humans and animals with dynamic changes during the respiratory cycle. For the numerical flow simulations a twofold strategy has been employed, which on the one hand utilises a commercial package to investigate important parameters and boundary conditions. On the other hand a self-developed methodology on the basis of the Immersed Boundary method enables dynamic flow simulations. Both approaches have been successfully applied to natural and generic geometries, whereas the IB method allowed first insights to the oscillatory flow in dynamically deformed geometries, even though generic deformations were used here.

The results obtained are unique and prove the necessity of a three-dimensional dynamic method in order to extract the relevant flow physics. Based on this new information different ventilation strategies can be discussed. The self-developed method has been validated and a realistic parameter set has been obtained within the framework of presently available models. The initial analysis of the flow field revealed the existence of important vortex features and also the absence of streamwise separation so far.

Currently the developed methods are applied to the dynamic geometries acquired from the respiration period of artifical ventilated porcine airways (figure 4 right). The results of this dynamic flow simulation will allow to demonstrate the concept and to investigate the unsteady flow behaviour w.r.t. to natural geometry changes. The physics of the dynamic flow field will be examined and discussed in all detail for these simulations.

Although the workflow and the simulation code developed reached a robust state, a phase of improvements has been started recently in order to account for further realistic effects, e.g. lung impedance. The geometry segmentation will be enhanced by a likelihood estimation for small airways, and furthermore to extract deformation fields based on a non-rigid registration algorithm. This will allow to increase the segmentation depth and the accuracy of the extracted deformation fields. The numerical solution procedure will be incorporated by an adaptive mesh algorithm and lung impedance modelling.

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