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A Multiscale Bidirectional Coupling Framework

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Abstract—**The lung is geometrically articulated across multiple scales from the trachea to the alveoli. A major computational challenge is to tightly link ODEs that describe lower scales to 3D finite element or finite volume models of airway mechanics using iterative communication between scales. In this study, we developed a novel multiscale computational framework for bidirectionally coupling 3D CFD models and systems of lower order ODEs. To validate the coupling framework, a four and eight generation Weibel lung model was constructed. For the coupled CFD-ODE simulations, the lung models were truncated at different generations and a RL circuit represented the truncated portion. The flow characteristics from the coupled models were compared to untruncated full 3D CFD models at peak inhalation and peak exhalation. Results showed that at no time or simulation was the difference in mass flux and/or pressure at a given location between uncoupled and coupled models was greater than 2.43%. The flow characteristics at prime locations for the coupled models showed good agreement to uncoupled models. Remarkably, due to reuse of the Krylov subspace, the cost of the ODE coupling is not much greater than uncoupled full 3D-CFD computations with simple prescribed pressure values at the outlets.**

I. Introduction

It was shown as early as 1989 by Cohen et al. [1] that the presence of the distal lung affects the airflow in the proximal lung and the distal lung needs to be accounted in some way or form to accurately simulate flow distribution in the larger upstream airways. The most common boundary condition used at the outlets for a three-dimensional (3D) CFD simulation include uniform pressure, zero pressure or a constant mass flow boundary condition assuming the lung to be uniformly ventilated [2]. Though, this assumption might hold good at low ventilation frequency, it is not true at high frequency ventilation, where the ventilation in the lung has been shown to be heterogenous in nature [3]. Therefore, most of the computational models involving respiratory system have applied boundary conditions that do not reflect the presence of the distal lung. This can be attributed to the sheer complexity of the animal/human tracheobronchial tree and lack of available data. The very reason, the multiscale paradigm, wherein 3D distributed finite-element or finite-volume models, are coupled with lower-dimensional ordinary differential equation (ODE) or partial differential equation (PDE) representing the distal lung mechanics has attracted considerable attention in the respiratory modeling community.

For multiscale modeling, the current state of the art is an integrated monolithic approach, wherein the 3D and the ODE/PDE models are consistently discretized and solved for simultaneously [4]. From a mathematical point of view, this process is rigorous, but requires a dedicated solver and considerable numerical sophistication by the user. There is no doubt that this method is optimal for the lower dimensional systems that can be consistently discretized.

A less demanding, but also less accurate, approach is to perform unidirectional coupling between the 3D distributed model and the lower-dimensional model. For example, Ma et. [5] have investigated the flow characteristics and deposition pattern in the human upper and central airways. The geometry consisted of a 3D model of the upper airway based on Magnetic Resonance (MR) images and anatomically based 3D model of the central airways reconstructed from Computed Tomography (CT) images. A one-dimensional (1D) transmission line model was adopted to represent the distal airway tree that accounted for the impedance of the small airways. The electrical representation of the distal airway tree was coupled to the outlets of the 3D model for supplying the boundary conditions necessary for the CFD simulation. A major limitation of this study was that the coupling of the 1D and 3D models were unidirectional i.e., the impedance from the 1D model was imposed at the outlets of the 3D model, not accounting for the probable changes in the impedance in the 1D model due to changes encountered in mass flux at the corresponding outlet of the 3D model after every timestep.

To overcome these challenges, we present a novel partitioned, multiscale computational framework for iteratively coupling multiple boundary interfaces, with an

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efficiency that is close to that of the monolithic methods, but that offers greater flexibility in terms of enabling the coupling of existing finite element or finite volume solvers, without consistent discretization between higher-dimensional and lower-dimensional systems.

To validate the multiscale-coupling framework, truncated four- and eight-generation Weibel lung models were coupled to resistor-inductor (RL) circuits. Pressure, mass flux and regional flow characteristics from the coupled models were compared to full 3D CFD models at prime locations during peak inhalation and peak exhalation.

II. Materials and Methods

A. Multiscale Coupling Framework

For the coupling to work, the pressure at the interface between the 3D model and the ODE model has to be determined. This pressure will determine the flow in the 3D and the ODE system. Our task is to determine the interface pressure at each CFD timestep for each outlet, such that the flow in the 3D system and the ODE system match within a numerical tolerance.

The most straightforward approach is to use Newton's method. However, this method is very expensive when the number of outlets is large. This is because every coupled outlet requires a separate CFD evaluation. To avoid this, Miller devised a 'Nonlinear Krylov accelerator' or the 'modified Newton's method' [6]. We extended the nonlinear Krylov accelerator *"NACCEL"* for accelerating Newton iterations and further reduced cost by eliminating explicit evaluation of the Jacobian matrix; instead, we implicitly accumulated and updated the Jacobian information on the active Krylov subspace over multiple time steps.

NACCEL was implemented as a C++ boundary class in OpenFOAM (OpenCFD Ltd, Reading, UK). The sole inputs to the accelerator are the outlet residuals. The output consists of a pressure correction to be applied to the CFD boundary.

B. Weibel Lung Geometry

OSO (OSO, developed at Los Alamos National Laboratory and CGC) was used to generate the surfaces pf the Weibel lung models. Further details about the surface generation can be found in [2]. Lagrit-PNNL was used to constrain, smooth and adapted the surface mesh [7]. Gambit (Fluent, Lebanon, NH) was used to convert the final surface geometry to an unstructured volume mesh mainly consisting of tetrahedral elements.

C. Transmission Line Model

The resistance of an airway for the CFD-ODE model was approximated to the resistance for steady laminar pipe flow (Poiseuille flow), which is independent of the frequency.

$$R = \frac{8\mu}{\pi r^4}$$

where R is the resistance per unit length of the airway, r is the radius of the airway, and μ is dynamic viscosity of air. The inductance of an airway was computed using the original transmission line formula based on the approximations given by Keefe [8].

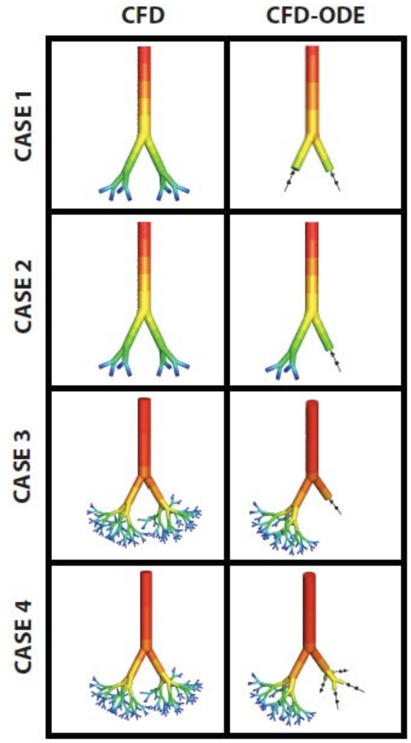

Fig. 1. Four different cases were studied to validate the CFD-ODE coupling methodology.

$$L = \frac{4\rho}{3\pi r^2}$$

where L is inertance per unit length, ρ is the density and r is the radius of the airway. For calculating the resistances and inductances, the lengths and radii of the airways were obtained from the Weibel morphometry.

At very low Reynolds number such as in the current study, the ratio of actual energy dissipation (which includes the bifurcational loss) to the energy dissipation predicted by the Poiseuille flow resistance is less than or equal to one [9]. This suggests that the energy loss at bifurcation is negligible and hence resistance and inductance of the bifurcations in the ODE system was neglected.

D. Numerical Methods

The airflow predictions were based on the laminar three-dimensional, incompressible Navier-Stokes equations for fluid mass and momentum. An adaptive time-stepping algorithm was utilized for the selection of optimum time step. The algorithm adjusted the time step so as to limit the Courant number to be less than 0.5. For all calculations, air at room temperature was considered to be the working fluid, with a density of 1.0 kg/m^3 and a kinematic viscosity of 1.502e-05 m^2/s. The trachea/inlet was assigned zero pressure for all the models. All outlets were prescribed a pressure sine wave mimicking inhalation and exhalation. No-slip condition was applied to the remaining airway boundaries. Airflow was assumed to be laminar on the basis of computed Reynolds number at peak inhalation and peak exhalation.

E. Validation

To validate the coupling methodology, four different cases (see figure 1) based on the Weibel lung model were studied:

– Case 1: a 4-generation CFD model was compared to a 2-generation CFD-ODE model.

– Case 2: a 4-generation CFD model was compared to an asymmetrical model in which the left bronchus was chopped and RL circuits represented generations 3 and 4.

– Case 3: a 8-generation CFD model was compared to an asymmetrical model in which the left bronchus was chopped and RL circuits represented the distal airways up to 8 generation.

– Case 4: a 8-generation CFD model was compared to an asymmetrical model in which the left lung was chopped at the 4th generation and RL circuits represented the distal airways up to 8 generation.

Boundary conditions consisted of a fixed atmospheric pressure at the trachea, and a sinusoidal pressure applied at the outlets of the un-truncated 3D model and at the ends of the individual ODE circuits.

For each of these cases, the flow fields at the end of the trachea, right and left bronchus (figure 2) from the coupled models were compared to uncoupled models at peak inhalation and peak exhalation.

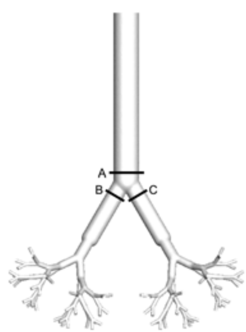

Fig. 2. Locations selected for probing the flow characteristics.

F. Outlet Independence Study

In addition to the four cases studied for validation, all the outlets in the un-chopped 4-generation Weibel lung model were coupled to ODEs representing the distal lung up to 23 generations. This study was performed to investigate the relative independence of the coupling algorithm to the number of coupled outlets.

G. Mesh Convergence

To verify that the solution was independent of the mesh, the mesh density was approximately doubled. Otherwise, same boundary conditions and solution parameters were used. Pressure and mass flux were compared at three main locations: 1) end trachea, 2) right bronchus and 3) left bronchus.

III. Results

A. Mesh Convergence

At the locations for comparison, there was no noticeable variation in the axial velocity contours or in the secondary radial velocity. This was true at both peak inhalation and peak exhalation. Because the time step is estimated by the Courant condition and the difference between the solutions of two different meshes is negligible, we infer that the solution is independent of mesh and time step.

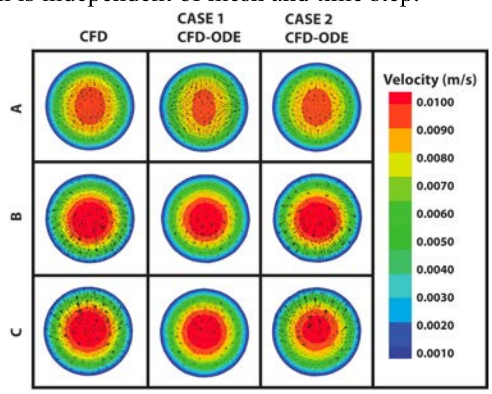

Fig. 3. Contours of velocity magnitude and vectors showing secondary flows at **peak inhalation** for the CFD and CFD-ODE Cases 1 & 2 (see Figures 1 and 2). The results are remarkably similar between each coupled and uncoupled case and the 3D CFD result.

B. Validation

For all the cases, there was good correspondence between the results of the CFD and CFD-ODE simulations, both in terms of absolute velocity and secondary flow during both peak inhalation (see figure 3 & 5; only peak inhalation shown) and peak exhalation. Below are the results for mass flux, pressure and iteration history:

Case 1: There was a 1.35% difference in mass flux (at peak exhalation) and a 2.43% difference in pressure (at peak inhalation) at any time during the breathing cycle. In most cases only a single CFD evaluation was necessary (Figure 4). Specifically, 77.7% of the timesteps required only a single CFD call, while 22% of the timesteps required two

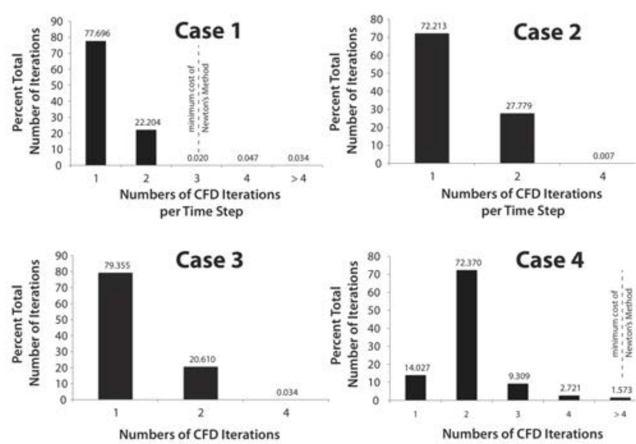

Fig. 4. Number of CFD iterations per timestep for each of the four cases. Note that in the first three cases approximately 3/4 of all timesteps required only a single CFD evaluation, while the remaining approximately 1/4 of all timesteps only required two CFD evaluations.

CFD calls. The fraction that remained occurred at the zero crossing between inhalation and exhalation.

Case 2: There was 0.56% difference in mass flux (near peak exhalation) and a 0.86% difference in pressure (at peak inhalation) for the entire inhalation and exhalation phase. Majority of the timesteps (72.2%) required only a single CFD call, while 27.8% of the timesteps required two CFD calls (figure 4). A single timestep required four CFD calls and occurred near zero crossing.

Case 3: The maximum difference in mass flux at any time during the breathing cycle was 2.13% and occurred at peak exhalation. Similarly, the maximum percentage difference in pressure was 1.18% at peak inhalation. More than 75% of the timesteps required just single CFD call and the remaining timesteps required two CFD calls.

Case 4: The maximum difference in mass flux was 1.35% at peak exhalation and 2.43% in pressure at peak inhalation

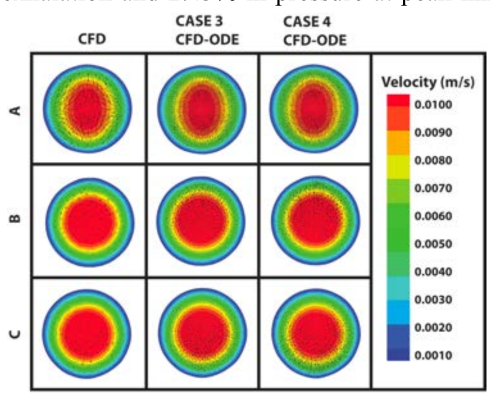

Fig. 5. Contours of velocity magnitude and vectors showing secondary flows at **peak inhalation** for the CFD and CFD-ODE Cases 3 & 4

for the entire breathing cycle. For 14% of the timesteps, a single CFD evaluation was required. The majority of the remaining timesteps (69%) required two CFD calls. The remaining timesteps required greater than four CFD calls.

C. *Outlet Independence Study*

Majority (67.8%) of the timesteps required two CFD calls. The remaining timesteps required 3-10 CFD evaluations per timestep.

IV. Discussion and Conclusion

We have presented a novel bidirectional coupling framework for iteratively coupling 3D models to lower order models representing the distal lung mechanics. The approach is an extension of the nonlinear Krylov accelerator introduced by Carlson and Miller [6].

The multiscale framework was validated using coupled models of the Weibel lung. For the CFD-ODE models a system of ODE's describing the distal airway tree in terms of resistance, and inductance based on the Weibel morphometry were coupled to truncated 3D outlets.

In all cases, the coupled solution was able to recover the behavior of the full system, with an average error in mass flux of 0.97% and an average error in pressure of 1.11%.

For Cases 1, 2 and 3, between 72% and 80% of the timesteps required only a single CFD-ODE evaluation. It should be noted that a standard Newton's Method would have required at a theoretical minimum the same number of residual evaluations, as there are coupled outlets. Most of the iterations for case 4 required two CFD calls. This could be attributed to the fact that there could be a feedback mechanism between the coupled outlets because of their proximity. Extrusion of the outlets should help minimize this effect.

The relative independence of the coupling algorithm to the number of coupled outlets was demonstrated using the *"Outlet Independence Study"* in which most of the iterations required two CFD calls.

The Krylov accelerator was implemented as a C++ boundary class in OpenFOAM. This boundary class can be easily adapted to other commercial and open source solvers where in the user has access to the inner iterations.

V. Limitations and Future work

Though the relative independence of the method on the number of coupled outlets was implicitly illustrated using the *"Outlet Independence Study"*, more rigorous testing is warranted. Realistic geometry based on MRI/CT data is being considered for future work.

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