

An immersed boundary method for patient-specific modelling of flow and aerosol deposition in the respiratory airways

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SUMMARY

An immersed boundary (IB) method for patient-specific modelling of flow in the respiratory airways is presented. No-slip conditions are enforced via momentum forcing and mass conservation at immersed boundaries is satisfied via a mass source term developed for moving walls. An iterative scheme to compute the forcing term implicitly reduces the errors at the boundary and enhances stability. In addition, the mass source term accurately accounts for airway movement during breathing, and reduces the spurious force oscillations which typically arise in IB simulations of moving body problems. The method is developed for use in a generalised curvilinear system, which is particularly useful in bioflow problems involving complex geometries. Flow in realistic extrathoracic airways is examined with this method.

Key Words: *immersed boundary, moving boundaries, curvilinear, respiratory airways.*

1 INTRODUCTION

Understanding the flow dynamics in the respiratory system is important in determining the efficiency of aerosolized drug delivery and the toxicity of airborne pollutants. Accurate and efficient prediction poses a challenge due to the complexity of the flow in the airways and the complexity of the airway geometries. Due to the bifurcating nature of the lung and the effect of the breathing cycle on the flow, patterns in the respiratory airways are complex even during quiet breathing. The flow remains turbulent in the mouth and throat and the larger airways, before extensive branching increases the total cross-sectional area and therefore reduces the gas velocity through each airway, causing laminarisation. In most of the tracheobronchial tree, the flow is intermittently turbulent with eddies forming at the branching points. Accurate solution of the flow field therefore motivates the use of direct numerical simulations (DNS) in order to resolve all the scales in the flow. Due to the high grid resolution requirements, it is desirable to adopt an efficient computational strategy. To this end, an immersed boundary method for curvilinear coordinates is developed, which allows the use of structured grids to model the complex patient-specific airways. Use of structured grids greatly simplifies the task of grid generation, particularly for moving airway boundaries and circumvents the need for remeshing at every time step which leads to more efficient computational algorithms. Compared to a Cartesian grid, curvilinear grids can further improve efficiency by minimising the number of grid points outside the fluid domain, can have a more natural alignment with the streamlines which is desirable for the accuracy of the solution, and can provide a better wall-normal resolution.

2 NUMERICAL METHOD AND RESULTS

The no-slip condition at the immersed boundary (i.e. the airway walls) is applied via a direct forcing approach, which consists in adding a momentum forcing term, f , on the boundary and outside the lung geometry. The forcing ensures that the velocity at the airway walls satisfies the boundary conditions. A mass source/sink, q , is applied to cells containing the immersed boundary in order to ensure mass conservation. The equations are discretized on a staggered curvilinear grid using a finite volume scheme, following the method described in [1]. Time integration is performed using a second-order fractional step method. The diffusive terms are treated implicitly

using the Crank-Nicolson scheme and the non-linear convective terms are treated explicitly using an Adams-Bashforth scheme. The discretized equations are given by

$$\frac{\hat{\mathbf{u}} - \mathbf{u}^{n-1}}{\Delta t} = -(\gamma N(\mathbf{u}^{n-1}) + \delta N(\mathbf{u}^{n-2})) - \nabla p^{n-1} + \frac{1}{Re} (\alpha L(\hat{\mathbf{u}}) + \beta L(\mathbf{u}^{n-1})) + \mathbf{f}^n \quad (1)$$

$$\nabla^2 \phi^n = \frac{1}{\Delta t} (\nabla \cdot \hat{\mathbf{u}} - q^n) \quad (2)$$

$$\mathbf{u}^n = \hat{\mathbf{u}} - \Delta t \nabla \phi^n \quad (3)$$

$$p^n = p^{n-1} + \phi^n \quad (4)$$

where $N(\mathbf{u})$ are the convective terms, $L(\mathbf{u})$ are the implicit diffusive terms and $(\alpha, \beta, \gamma, \theta)$ are weighting coefficients which depend on the numerical scheme adopted. In our case, $\alpha = 3/2$, $\beta = -1/2$ for the Adams-Bashforth scheme and $\gamma = \theta = 1/2$ for the Crank-Nicolson scheme.

2.1 Momentum forcing term

The accuracy and stability of direct forcing methods used in conjunction with the fractional step algorithm depend on the computation of the forcing term. In the semi-implicit fractional step method, the velocities and forcing terms are coupled through the implicit diffusive terms. Kim et al. [2] proposed a solution which consisted in provisionally advancing the velocity field explicitly in order to compute the forcing term and then adding it to the semi-implicit momentum equations. However, this scheme introduces errors near the immersed boundary as the velocities are advanced implicitly but the forcing term is calculated explicitly. The error due to the explicit treatment of the diffusive terms in the calculation of \mathbf{f}^n can render the scheme unstable in two scenarios: (i) the low-Reynolds-number flow in the terminal bronchioles; (ii) the turbulent flow in the extrathoracic airways where near-wall resolution can render the viscous stability constraint more restrictive.

The solution proposed herein consists in splitting the intermediate velocity equation into two steps,

$$\frac{\tilde{\mathbf{u}} - \mathbf{u}^{n-1}}{\Delta t} = \frac{1}{Re} (\alpha L(\tilde{\mathbf{u}}) + \beta L(\mathbf{u}^{n-1})) - G p^{n-1} - \gamma N(\mathbf{u}^{n-1}) - \theta N(\mathbf{u}^{n-2}) + \mathbf{f}^{n-1} \quad (5)$$

$$\frac{\hat{\mathbf{u}} - \tilde{\mathbf{u}}}{\Delta t} = \frac{\alpha}{Re} (L(\hat{\mathbf{u}}) - L(\tilde{\mathbf{u}})) + \delta \mathbf{f}^n, \quad (6)$$

which fully recovers Eq. 1. In the first step, an approximation, $\tilde{\mathbf{u}}$, of the intermediate velocity is determined. This velocity field does not satisfy the exact boundary conditions at the immersed boundary since the forcing applied is evaluated from the previous time step. In the second step, the forcing is updated and the no-slip constraint at the immersed boundary is satisfied. The exact expression for $\delta \mathbf{f}^n$ is obtained from Eq. 6 by applying the no-slip constraint at the immersed boundary ($\hat{\mathbf{u}} = \mathbf{u}_{IB}^n$ at IB points):

$$\delta \mathbf{f}^n = \frac{\mathbf{u}_{IB}^n - \tilde{\mathbf{u}}}{\Delta t} - \frac{\alpha}{Re} (L(\hat{\mathbf{u}}) - L(\tilde{\mathbf{u}})). \quad (7)$$

Since the diffusive term, $L(\hat{\mathbf{u}})$, in Eq. 7 is unknown, an iterative method is required to solve for $\hat{\mathbf{u}}$ and $\delta \mathbf{f}^n$ implicitly. The first term in the forcing (Eq. 7) drives the velocity at the boundary to the target value (i.e. it enforces the no-slip boundary constraint) while the second term ensures that the diffusive term at the boundary and, hence, the velocities $\hat{\mathbf{u}}$ at surrounding non-IB points are correct. Compared to the explicit forcing method, the implicit approach remains stable up to approximately 2.5 times larger Δt . The second-order accuracy of the scheme in both space and time is demonstrated in fig. 1 using the standard decaying vortex test case [2].

2.2 Mass source term for moving boundaries

Application of IB methods to moving boundary problems can lead to spurious force oscillations (SFOs) due to the violation of local mass conservation [3,4]. In the present method, an extension of the mass source term by Kim et al. [2] for use with moving boundaries is proposed in order to

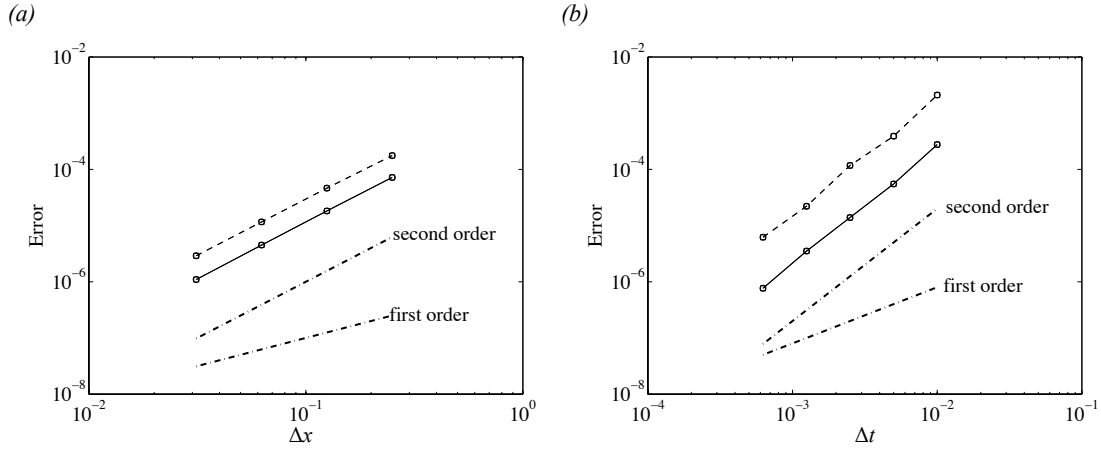


Figure 1: L_2 (—) and L_∞ (- - -) norms for the u (\square) and v (\circ) velocities versus (a) grid spacing, and (b) time step for decaying vortex problem at $Re = 500$.

satisfy mass conservation near the boundary and suppress SFOs. The present mass source term is designed to enforce local and global mass conservation and is given by

$$q^n = \frac{1}{\Delta V} \left(\sum_{i=1}^6 \beta_s \hat{\mathbf{u}} \cdot \mathbf{n} \Delta S_i + \mathbf{u}_\Gamma^n \cdot \mathbf{n}_\Gamma \Delta \Gamma \right), \quad (8)$$

where ΔV is the cell volume, ΔS_i is the area of each cell face, \mathbf{n} is the unit normal vector outward at each cell face and β_s is the fraction of the cell face inside the solid. The quantities u_Γ , n_Γ and $\Delta \Gamma$ are the surface velocity, the surface outward unit normal vector (pointing towards the fluid), and the area of the boundary within the cell, respectively.

The first term on the right-hand-side of Eq. 8 mimics the cut-cell/virtual cell-merging technique [3] without requiring construction of new polyhedral cells. It ensures that the continuity equation is satisfied for the fraction of the cell inside the fluid by excluding the contribution from outside the lung geometry. Since two neighbouring cells which share a common face have the same value of the surface flux, but with opposite signs, the global contribution of this term vanishes [2]. The second term in Eq. 8 is an addition to the original mass source term, and ensures that the continuity equation is satisfied when the boundary is moving by including the flux at the boundary. Figure 2 demonstrates the ability of the proposed mass source term to suppress spurious force oscillations in a moving body problem.

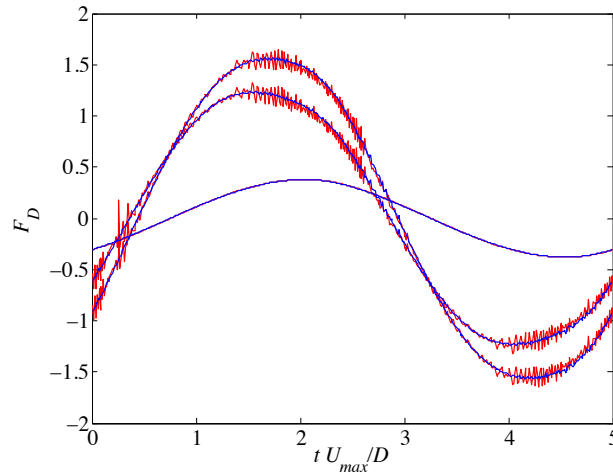


Figure 2: Temporal evolution of drag force on an oscillating cylinder at $Re_{\max} = 100$: —, momentum forcing without a mass source; —, momentum forcing with a mass source.

2.3 Flow in the extrathoracic airways

The new IB method has been applied to perform the first set of fully-resolved simulations of the flow in realistic extrathoracic airways [5]. Through realistic geometric representation of the airways and detailed flow fields, the effect of geometric variation on the mean flow as well as the

turbulent fluctuations has been studied. Comparison of the main flow features with PIV measurements in the same geometries [6] shows good agreement with our numerical predictions. Figure 3 shows the grid, flow field and deposition pattern in one of these geometries. The velocity profiles in the mouth are highly skewed towards the inner wall due to the airway curvature. The flow accelerates at the back of the mouth due to the restriction in cross-sectional area, developing a pharyngeal jet which impinges onto the posterior wall. Due to the bend in the airway, the flow shifts towards the outer wall, separating from the inner wall and leading to a recirculation region (fig. 3*b*). The maximum kinetic energy occurs in the upper pharynx near the jet (fig. 3*c*). The flow field has a large effect on the particle deposition as can be observed in fig. 3*d*. A deposition hot-spot is observed at the posterior wall of the upper pharynx where particles deposit via impaction due to the pharyngeal jet. The method is currently being applied to the intrathoracic airways, taking into account the airway movement during the breathing cycle.

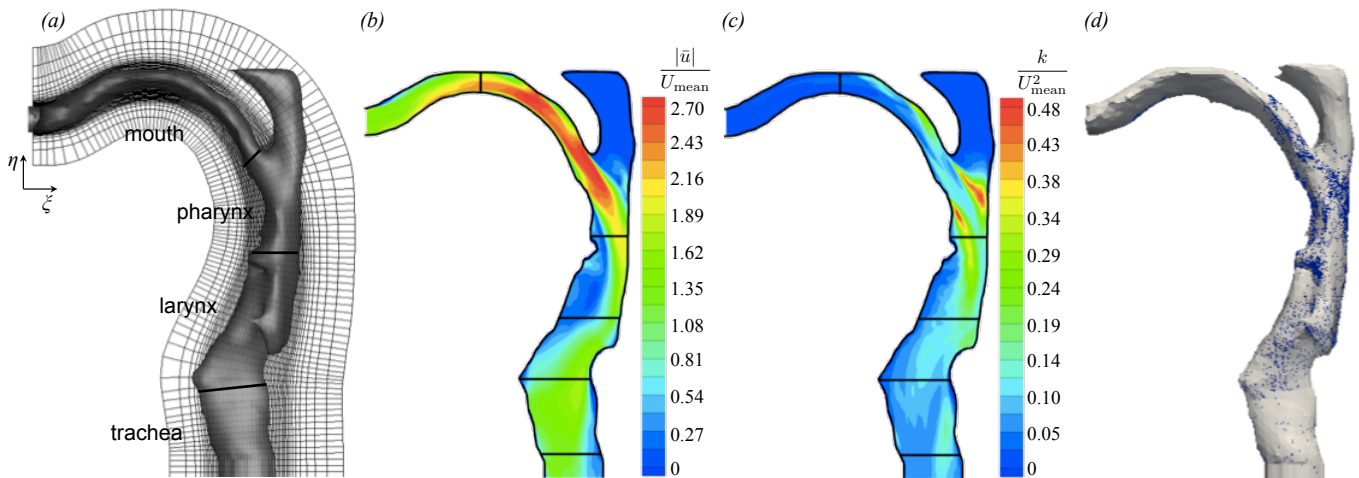


Figure 3: Flow in realistic extrathoracic airways. (a) Airway geometry and curvilinear grid (every eighth grid line in ξ and η is plotted); (b) mean velocity magnitude; (c) mean turbulent kinetic energy; (d) particle deposition.

3 CONCLUSIONS

An immersed boundary method for patient-specific simulations of flow in the respiratory airways has been presented. The implicit iterative scheme decreases the errors at the boundary and enhances stability. The method can also be applied in generalized curvilinear coordinates for efficient modelling of the complex airway geometries. Finally, the new mass source term improves local mass conservation at moving geometry walls and suppresses spurious force oscillations. The method has been applied for detailed simulations of the turbulent flow in realistic extrathoracic airways.

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