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Developing computational methods for three-dimensional finite element simulations of coronary blood flow

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ABSTRACT

Coronary artery disease contributes to a third of global deaths, afflicting seventeen million individuals in the United States alone. To understand the role of hemodynamics in coronary artery disease and better predict the outcomes of interventions, computational simulations of blood flow can be used to quantify coronary flow and pressure realistically. In this study, we developed a method that predicts coronary flow and pressure of three-dimensional epicardial coronary arteries by representing the cardiovascular system using a hybrid numerical/analytic closed loop system comprising a three-dimensional model of the aorta, lumped parameter coronary vascular models to represent the coronary vascular networks, three-element Windkessel models of the rest of the systemic circulation and the pulmonary circulation, and lumped parameter models for the left and right sides of the heart. The computed coronary flow and pressure and the aortic flow and pressure waveforms were realistic as compared to literature data.

1. Introduction

Computational simulations have become a useful tool in studying blood flow in the cardiovascular system [37], enabling quantification of hemodynamics of healthy and diseased blood vessels [7,22,36], design and evaluation of medical devices [17,34], planning of vascular surgeries, and prediction of the outcomes of interventions [19,31,38]. Much progress has been made in computational simulations of blood flow as the computing capacity and numerical methods have advanced. In particular, more realistic boundary conditions have been developed in an effort to consider the interactions between the computational domain and the absent upstream and downstream vasculatures considering the closed loop nature of the cardiovascular system. These boundary conditions represent the upstream and downstream vasculatures using simple models such as resistance, impedance, lumped parameter models, and one-dimensional models and couple to computational models either explicitly or implicitly [9,14,19,24,42].

These boundary conditions can be utilized to quantify flow and pressure fields in the epicardial coronary arteries. However, unlike other parts of the cardiovascular system, prediction of coronary blood flow exhibits greater complexity because coronary flow is influenced by the contraction and relaxation of the ventricles in addition to the interactions between the computational domain and the absent upstream and downstream vasculatures. Unlike flow in other parts of the arterial system, coronary flow decreases in systole when the ventricles contract and compress the intramyocardial coronary vascular networks and increases in diastole when the ventricles relax. Thus, to model coronary flow realistically, we need to consider the compressive force of the ventricles, which causes the intramyocardial pressure, acting on the coronary vessels throughout the cardiac cycle.

Most previous studies on coronary flow and pressure using three-dimensional finite element simulations ignored the intramyocardial pressure, and prescribed, not predicted, coronary flow. Further, these studies generally used traction-free outlet boundary conditions [2,3,11,20,21,23,25,27,32,43,47,48] and did not compute realistic pressure fields. Migliavacca et al. [15,19] computed three-dimensional pulsatile coronary flow and pressure in a single coronary artery by considering the intramyocardial pressure but this study was performed with an idealized model and low mesh resolution. Additionally, the analytic models used as boundary conditions were coupled explicitly, necessitating either sub-iterations within the same time step or a small time step size bounded by the stability of an explicit time integration scheme. To predict physiologically realistic flow rate and pressure in the coronary arterial trees of a patient, computational simulations should be robust and stable enough to handle complex flow

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characteristics, and the coupling should be efficient and versatile with different levels of mesh refinement [13].

In this paper, we describe methods to calculate flow and pressure in three-dimensional coronary vascular beds by considering a hybrid numerical/analytic closed loop system. For each coronary outlet of the three-dimensional finite element model, we coupled a lumped parameter coronary vascular bed model and approximated the impedance of downstream coronary vascular networks not modeled explicitly in the computational domain. Similarly, we assigned Windkessel models to the upper branch vessels and the descending thoracic aorta to represent the rest of the systemic circulation. These outlets feed back to the heart model representing the right side of the heart and travel to the pulmonary circulation, which is approximated with a Windkessel model. For the inlet, we coupled a lumped parameter heart model that completes a closed-loop description of the system. Using the heart model, it is possible to compute the compressive forces acting on the coronary vascular beds throughout the cardiac cycle. Further, we enforced the shape of velocity profiles of the inlet and outlet boundaries with retrograde flow to minimize numerical instabilities [13]. We solved for coronary flow and pressure as well as aortic flow and pressure in subject-specific models by considering the interactions between these model of the heart, the impedance of the systemic arterial system and the pulmonary system, and the impedance of coronary vascular beds.

2. Methods

2.1. Three-dimensional finite element model of blood flow and vessel wall dynamics

Blood flow in the large vessels of the cardiovascular system can be approximated by a Newtonian fluid [22]. In this study, we solved blood flow using the incompressible Navier–Stokes equations and modeled the motion of the vessel wall using the elastodynamics equations [8].

For a fluid domain Ω with boundary Γ and solid domain Ω^s with boundary Γ^s, we solve for velocity $\vec{v}(\vec{x},t)$, pressure $p(\vec{x},t)$, and wall displacement $\vec{u}(\vec{x}^s,t)$ [8,41] as follows:

Given $\vec{f}:\Omega\times(0,T)\to\mathbb{R}^3$, $\vec{f}^s:\Omega^s\times(0,T)\to\mathbb{R}^3$, $\vec{g}:\Gamma_g\times(0,T)\to\mathbb{R}^3$, $\vec{g}^s:\Gamma^s_g\times(0,T)\to\mathbb{R}^3$, $\vec{v}_0:\Omega\to\mathbb{R}^3$, $\vec{u}_0:\Omega^s\to\mathbb{R}^3$, and $\vec{u}_{0,t}:\Omega^s\to\mathbb{R}^3$, find $\vec{v}(\vec{x},t)$, $p(\vec{x},t)$, and $\vec{u}(\vec{x}^s,t)$ for $\forall\vec{x}\in\Omega$, $\forall\vec{x}^s\in\Omega^s$, and $\forall\, t\in(0,T)$, such that the following conditions are satisfied:

$$\rho\vec{v}_{,t}+\rho\vec{v}\cdot\nabla\vec{v}=-\nabla p+div(\underset{\sim}{\tau})+\vec{f}\quad\text{for }(\vec{x},t)\in\Omega\times(0,T)$$

$$div(\vec{v})=0\quad\text{for }(\vec{x},t)\in\Omega\times(0,T)$$

$$\rho^s\vec{u}_{,tt}=\nabla\cdot\underset{\sim}{\sigma}^s+\vec{f}^s\quad\text{for}(\vec{x}^s,t)\in\Omega^s\times(0,T)$$

where

$$\underset{\sim}{\tau}=\mu(\nabla\vec{v}+(\nabla\vec{v})^T)\quad\text{and}\quad\underset{\sim}{\sigma}^s=\underset{\sim}{C}:\tfrac{1}{2}(\nabla\vec{u}+(\nabla\vec{u})^T)\tag{1}$$

with the Dirichlet boundary conditions,

$$\vec{v}(\vec{x},t)=\vec{g}(\vec{x},t)\quad\text{for }(\vec{x},t)\in\Gamma_g\times(0,T)$$

$$\vec{u}(\vec{x}^s,t)=\vec{g}^s(\vec{x}^s,t)\quad\text{for }(\vec{x}^s,t)\in\Gamma^s_g\times(0,T)\tag{2}$$

the Neumann boundary conditions,

$$\vec{t}_{\vec{n}}=[-p\underset{\sim}{I}+\underset{\sim}{\tau}]\vec{n}=\vec{h}(\vec{v},p,\vec{x},t)\quad\text{for }\vec{x}\in\Gamma_h\tag{3}$$

and the initial conditions,

$$\vec{v}(\vec{x},0)=\vec{v}_0(\vec{x})\quad\text{for }\vec{x}\in\Omega$$

$$\vec{u}(\vec{x}^s,0)=\vec{u}_0(\vec{x}^s)\quad\text{for }\vec{x}^s\in\Omega^s$$

$$\vec{u}_{,t}(\vec{x}^s,0)=\vec{u}_{0,t}(\vec{x}^s)\quad\text{for }\vec{x}^s\in\Omega^s\tag{4}$$

For fluid–solid interface conditions, we use the conditions implemented in the coupled momentum method with a fixed fluid mesh assuming small displacements of the vessel wall [8].

The density ρ and the dynamic viscosity μ of the fluid, and the density ρ^s of the vessel walls are assumed to be constant. The external body force on the fluid domain is represented by $\vec{f}$. Similarly, $\vec{f}^s$ is the external body force on the solid domain, $\underset{\sim}{C}$ is a fourth-order tensor of material constants, and $\underset{\sim}{\sigma}^s$ is the vessel wall stress tensor.

We utilized a stabilized semi-discrete finite element method, based on the ideas developed by Brooks and Hughes [4], Franca and Frey [10], Taylor et al. [39], and Whiting et al. [44] to use the same order piecewise polynomial spaces for velocity and pressure variables.

2.2.. Boundary conditions

The boundary Γ of the fluid domain is divided into a Dirichlet boundary portion Γ_g and a Neumann boundary portion Γ_h. Further, we divide the Neumann boundary portion Γ_h into coronary surfaces $\Gamma_{h_{cor}}$, inlet surface Γ_{in}, and the set of other outlet surfaces Γ'_h, such that $\overline{(\Gamma_{h_{cor}}\cup\Gamma_{in}\cup\Gamma'_h)}=\Gamma_h$ and $\Gamma_{h_{cor}}\cap\Gamma_{in}\cap\Gamma'_h=\phi$. Note that for this study, when the aortic valve is open, the inlet surface is included in the Neumann boundary portion Γ_h, not in the Dirichlet boundary portion Γ_g to enable coupling with a lumped parameter heart model. Therefore, the Dirichlet boundary portion Γ_g only consists of the inlet and outlet rings of the computational domain when the aortic valve is open. These rings are fixed in time and space [8].

2.2.1. Boundary conditions for coronary outlets

To represent the coronary vascular beds absent in the computational domain, we used a lumped parameter coronary vascular model developed by Mantero et al. [18] (Fig. 1). The coronary venous microcirculation compliance was eliminated from the original model in order to simplify the numerics without affecting the shape of the flow and pressure waveforms significantly. Each coronary vascular bed model consists of coronary arterial resistance R_a, coronary arterial compliance C_a, coronary arterial microcirculation resistance $R_{a\text{-}micro}$, myocardial compliance C_{im}, coronary venous microcirculation resistance $R_{v\text{-}micro}$, coronary venous resistance R_v, and intramyocardial pressure $P_{im}(t)$.

For each coronary outlet $\Gamma_{h_{cor_k}}$ of the three-dimensional finite element model where $\Gamma_{h_{cor_k}}\subseteq\Gamma_{h_{cor}}$, we implicitly coupled the lumped parameter coronary vascular model using the continuity of mass and momentum operators of the coupled multidomain method [41] as follows:

$$\begin{aligned}
&[\underset{\sim}{M}_m(\vec{v},p)+\underset{\sim}{H}_m]\\
&=-\left(R\int_{\Gamma_{h_{cor_k}}}\vec{v}(t)\cdot\vec{n}\,d\Gamma+\int_0^t e^{\lambda_1(t-s)}Z_1\int_{\Gamma_{h_{cor_k}}}\vec{v}(s)\cdot\vec{n}\,d\Gamma\,ds\right)\underset{\sim}{I}\\
&\quad+\left(\int_0^t e^{\lambda_2(t-s)}Z_2\int_{\Gamma_{h_{cor_k}}}\vec{v}(s)\cdot\vec{n}\,d\Gamma\,ds-\vec{n}\cdot\underset{\sim}{\tau}\cdot\vec{n}\right)\underset{\sim}{I}+\underset{\sim}{\tau}-(Ae^{\lambda_1 t}+Be^{\lambda_2 t})\underset{\sim}{I}\\
&\quad-\left(\int_0^t e^{\lambda_1(t-s)}\cdot Y_1P_{im}(s)\,ds+\int_0^t e^{\lambda_2(t-s)}\cdot Y_2P_{im}(s)\,ds\right)\underset{\sim}{I}
\end{aligned}$$

$$[\vec{M}_c(\vec{v},p)+\vec{H}_c]=\vec{v}\tag{5}$$