# Simulation of Blood Flow in Arteries for Functional Assessment of Coronary Disease: Implementation of Numerical Code

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**Abstract.** Cardiovascular diseases (CVDs) are a global leading cause of death. Physiologically accurate simulations of blood flow in atherosclerotic coronaries has been a challenge for hospital implementation. This study innovates by implementing numerical code that models realistic and patient-specific flow in order to calculate the Fractional Flow Reserve (FFR). User-defined functions (UDFs) for outlet pressure boundary condition (Windkessel model) and viscoelastic behaviour of blood (sPTT model) were coded and implemented in ANSYS® Fluent 2023 software. This proof-of-concept study of two patients with a hemodynamic significant and insignificant stenosis in left coronary arteries (LCA) showed the numerical and invasive FFR values differed by relative errors of around 12%. For Patient 1 (hemodynamic significant stenosis), the invasive FFR is 0.58, and the numerical FFR is 0.50. For Patient 2 (hemodynamic insignificant stenosis), the invasive FFR is 0.81 and the numerical FFR is 0.90. This study highlights the blood flow representation in hemodynamic simulations and this FFR calculation tool offers a promising, fast, accurate, no costs, and non-invasive assessment of atherosclerotic disease in patients. After further validation with more patient cases, it could be used in hospitals my medical doctors and aid the diagnosis and treatment of CVDs.

**Keywords:** Numerical Methods, Coronary Artery Hemodynamics, Fractional Flow Reserve.

## 1 Introduction

Cardiovascular diseases are a major cause of mortality and morbidity in developed countries [1]. Coronary atherosclerotic disease (CAD) is a degenerative process that is characterized by the development of atheromatous plaques on the wall of coronary arteries. Clinical manifestations of CAD range from stable angina, resulting from progressive plaque growth with partial obstruction of the arterial lumen (stenosis) and consequent limitation of coronary blood flow. In clinical practice, a diagnostic strategy is widely used to assess the functional relevance of CAD: the invasive assessment of myocardial fractional flow reserve (FFR).

Coronary Computed Tomography Angiography (CTA) is an established non-invasive diagnostic tool for evaluating CAD. However, CTA can overestimate anatomic stenosis and is limited in that it does not provide information on the hemodynamic relevance of coronary stenosis. Thus, the implementation and numerical simulation of blood flow in arteries in the most real physiological conditions has been one of the main areas of interest of the authors [2]. The main purpose of this work is to develop and validate a computational tool for calculating the FFR and hemodynamic descriptors.

In this way, to obtain the most accurate non-invasive FFR, the hemodynamic numerical tool was hardly improved to establish real conditions, specific to each patient case with CAD. Therefore, to achieve accurate pressures,

Windkessel models, mainly based on the resistance of blood flow [3], were implemented considering hyperemia conditions (maximal dilation of the coronary tree), since the patient must be subjected to this condition during the catheterization to obtain the invasive FFR (reference value for validation). Moreover, the 3D patient-specific geometry of the artery was modified to simulate blood flow in hyperemic conditions. The numerical code development was performed in ANSYS® software.
After validation, the authors aim to create a software for local use, allowing a comprehensive assessment of CAD in an accessible, fast, reliable, and non-invasive way.

# 2 Methodology

A database of patients provided by Vila Nova de Gaia/Espinho Hospital Centre (CHVNG/E) has been used. In this study, hemodynamic and FFR results are presented for two patient cases: Patient 1 and Patient 2. However, the methodology will be presented only for Patient 1. The methodology used is the same for Patient 2.

## 2.1 Geometry reconstruction

The 3D model of the patient-specific geometry, under resting conditions, was reconstructed through Mimics® software and based on the Computed Tomography (CT) scans of the patient (Fig. 1) [4, 5]. Since the invasive FFR of the patient was measured in hyperemia conditions, induced by the intravenous administration of adenosine, the geometry for the computed FFR must be in the same conditions. Thus, the model of the patient geometry was enlarged by a factor of 2.04 of the cross-sectional area of the artery. Solidworks® software was used to finalize the geometry with the boundary conditions (Fig. 2). After this step, the geometry of the patient-specific artery is ready to use in hemodynamic simulations.

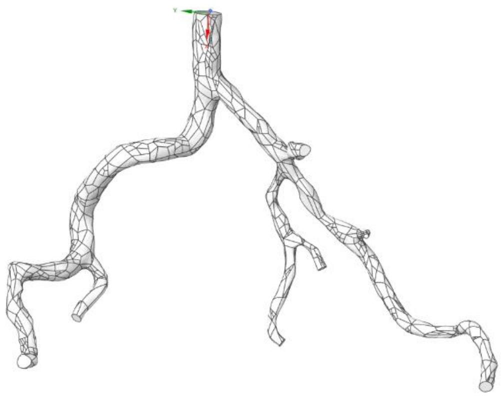

Figure 1. Model of the Patient Coronary Artery under Resting Conditions.

Figure 2. Model of the Patient Coronary Artery under Maximum Hyperemia Conditions.

### 2.2 Mesh construction

The mesh of the patient-specific coronary artery was constructed using Meshing Ansys® software. The Path Independent Method was used in order to uniform the mesh element size. The accuracy of the mesh was studied combining the lower Maximum Skewness as possible and a reasonable computational time. The Maximum Skewness is the most relevant metric to achieve an accurate mesh, and following the tutorial guide of Ansys® [6], it must be lower than 0.9. The Maximum Skewness was 0.61174 for Patient 1 and 0.6567 for Patient 2. Fig.3 shows the uniform and accurate mesh for Patient 1.

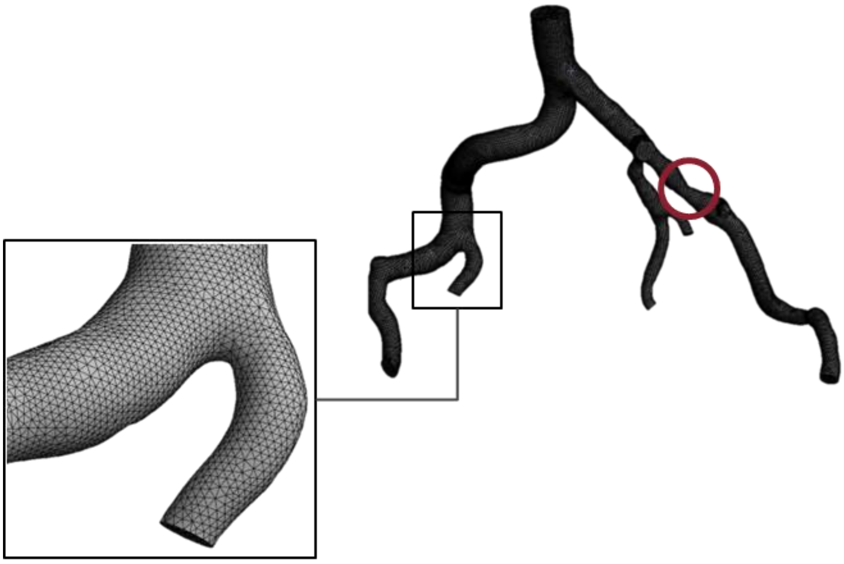

Figure 3. Computational Mesh of the Patient Coronary Artery.

### 2.3 Inlet boundary condition

At the inlet of the coronary artery, a Womersley velocity profile was used [4], depending on the time of the cardiac cycle ($t$), the position at the inlet ($r$) and the Womersley number ($\alpha$):

$$v(r,t) = 2.16\,\frac{AR^2}{\pi\mu\alpha^2}\left(1 - \frac{J_0\left(\alpha\,\frac{r}{R}\,i^{\frac{3}{2}}\right)}{J_0\left(\alpha\; i^{\frac{3}{2}}\right)}\right)e^{i\omega t} \tag{1}$$

$$\alpha = R\sqrt{\frac{\rho\omega}{\mu}} \tag{2}$$

$J_0$ is the Bessel function, $R$ the radius of the patient artery at the inlet and $A$ the respective cross-sectional area. $\mu$ is the mean viscosity of blood considered equal to 0.0035 Pa.s, ρ the constant density equal to 1060 kg/m$^3$ and $\omega$ the cardiac frequency of the patient. A User-Defined Function (UDF) was implemented in Ansys® software to mimic the inlet boundary condition specific for each patient. The Womersley numbers of Patient 1 and Patient 2 are 4.83 and 5.31, respectively.

### 2.4 Outlet boundary condition

At the outlet, a 3-element Windkessel model was used to simulate accurate pressure profiles specific for the patient [7]. This model is an analogy with an electrical circuit, for which the analytical component brings no issues, since the theory of electrical circuits is well developed. This model is governed by the following equations:

$$\frac{dp_d}{dt} + \frac{1}{C_a R_d} p_d = \frac{1}{C_a} Q_o \tag{3}$$

$$p_o = p_d + R_p Q_o \tag{4}$$

$R_p$ represents the proximal resistance, $R_d$ the distal resistance, $C_a$ the compliance, $Q_0$ the volume flow rate, $p_d$ the pressure at the arteriolar and capillary level and $p_0$ the pressure at the outlet. A UDF was implemented in Ansys® software for the outlets boundary conditions. A second-order implicit scheme was used for the discretization and the implementation accordingly to the Fluent Ansys® Theory Guide [8]:

$$p_o^{i+1} = \frac{Q_o^{i+1} + \frac{R_p C_a}{\Delta t}\left(\frac{3}{2} Q_o^{i+1} - 2Q_o^i + \frac{1}{2} Q_o^{i-1}\right) + \frac{C_a}{\Delta t}\left(2p_o^i - \frac{1}{2} p_o^{i-1}\right) + \frac{R_p}{R_d} Q_o^{i+1}}{\frac{3C_a}{2\Delta t} + \frac{1}{R_d}} \tag{5}$$

## 2.5 Rheology of blood

It is well known by the literature that blood is viscoelastic. The best model that represents these properties is the simplified Phan-Thien/Tanner (sPTT) [2]. This model was also implemented in UDFs coupled to the Fluent Ansys® solver, in order to solve the most real hemodynamic simulations of each patient.
The constitutive equations for this model are given by the following equations:

$$\boldsymbol{\tau} = \boldsymbol{\tau_s} + \boldsymbol{\tau_e} \tag{6}$$

$$\boldsymbol{\tau_s} = \mu_s \dot{\boldsymbol{\gamma}} \tag{7}$$

$$1 + \frac{\lambda \varepsilon}{\mu_e} tr(\boldsymbol{\tau_e})\boldsymbol{\tau_e} + \lambda \overset{\nabla}{\boldsymbol{\tau_e}} = \mu_e \dot{\boldsymbol{\gamma}} \tag{8}$$

$\boldsymbol{\tau_s}$ is the fluid contribution to the shear stress tensor, $\boldsymbol{\tau_e}$ is the elastic component contribution to the shear stress tensor, $\mu_s$ the suspending fluid viscosity, $\mu_e$ the elastic component viscosity, $\lambda$ the relaxation time, $\varepsilon$ the extensibility coefficient and $tr(\boldsymbol{\tau_e})$ represents the trace of the elastic shear stress tensor. The symbol $\nabla$ represents the upper-convected derivative.
The parameters of the multi-mode sPTT model for blood defined by Campo-Deaño et al. [9] were used, being represented in Table 1.

Table 1. Parameters used in the implementation of the sPTT model for blood. Adapted from [9].

| Mode (i) | $\mu_{e_i}$[Pa.s] | $\lambda_i$[s] | $\varepsilon_i$ |
|---|---|---|---|
| 1 | 0.05 | 7 | 0.2 |
| 2 | 0.001 | 0.4 | 0.5 |
| 3 | 0.001 | 0.04 | 0.5 |
| 4 | 0.0016 | 0.006 | 0.5 |
| Solvent | 0.0012 | 0 | 0 |

## 2.6 Numerical methodology

Fluent Ansys® software was used to run the hemodynamic simulations. The SIMPLE algorithm was used to solve the continuity and the momentum equations. A second-order implicit scheme was used to solve the pressure and velocity fields. A second-order upwind discretization scheme was used for the sPTT model. The artery walls were considered rigid, since the fluid-structure interaction (FSI) does not affect the results of hemodynamic simulations significantly and increases the computational cost [6].

### 2.7 Computed FFR

After running the hemodynamic simulations in Ansys® software, the FFR is calculated through the following equation:

$$FFR = \frac{p_d}{p_a} \tag{9}$$

$p_d$ is the distal pressure, at a distance of 20mm downstream from the stenosis; and $p_a$ is the aortic pressure, measured at a distance of approximately 10mm from the entrance to the coronary tree [10, 11]. The values for each pressure is the average pressure ($p_{avg}$) along the cardiac cycle. $T$ is the total time of the cardiac cycle and $P$ is the pressure value for each instant time.

After calculation, a computed FFR lower than 0.75 means a hemodynamically significant stenosis. If the FFR is higher than 0.80, the stenosis is insignificant. A FFR between 0.75 and 0.80 depends on the clinical decision.

$$p_{avg} = \frac{1}{T}\int_0^T P dt \tag{10}$$

## 3 Results and Discussion

Table 2 represents the computed FFR, obtained by the previous methodology, and the invasive FFR provided by CHVNG/E, for Patient 1 and Patient 2. Relative errors are also highlighted in the table.

Table 2. Computed and Invasive FFR for Patient 1 and Patient 2

| Patient | Computed FFR | Invasive FFR | Relative Error (%) |
|---|---|---|---|
| 1 | 0.58 | 0.497 | 14.3 |
| 2 | 0.81 | 0.904 | 11.6 |

Even though the error is high (>5%), the error is not considerably high (around 12% error). In addition, the comparison between the invasive and the computational FFR shows that the tool is able to correctly determine if the stenosis is mild or severe. In fact, Patient 1 has a hemodynamically significant stenosis (FFR < 0.75) and Patient 2 has a hemodynamically insignificant stenosis (FFR > 0.80), and the computational tool returned results in those ranges.

The decision of the medical doctors is the same based on the invasive or on the computational tool FFR. Therefore, for Patient 1, the procedure induces ischemia and requires revascularization. For the case of patient 2, the procedure does not induce ischemia and does not require revascularization.

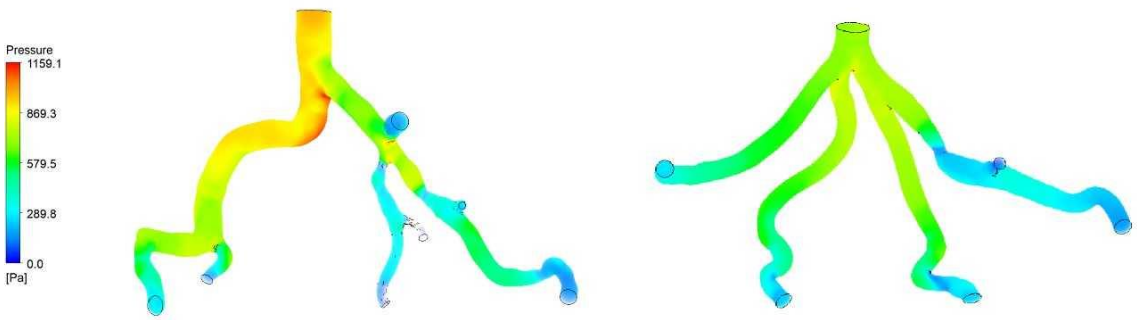


Figure 4. Pressure distribution at the systole phase of: a) Patient 1, b) Patient 2.

The figures of pressure distribution in the systole phase (Fig. 4) confirm that the stenosis of Patient 1 is hemodynamically significant and the FFR numerical value is low. The maximum pressure is 1159.1 Pa. For Patient 2, the FFR is high, so the pressure drop is not as significant as the other patient case. In fact, the maximum pressure of Patient 2 is lower than Patient 1, equal to 935.2 Pa.

# 4 Conclusions

In this work, two patient-specific 3D models of left coronary arteries were reconstructed using Mimics® software. Patient 1 has a hemodynamically significant stenosis and Patient 2 a hemodynamically insignificant one. The objective of the developed tool is to compute a numerical value of the FFR. The accuracy of the tool was assessed by comparing the computed FFR results with the non-invasive FFR value obtained invasively by medical doctors in the Vila Nova de Gaia/Espinho Hospital Centre. The invasive FFR values are taken as the points of reference for comparison with the numerical results. We have implemented numerical code through UDFs. Hemodynamic simulations were performed in Fluent Ansys® using the simplified Phan-Thien/Tanner rheological model to numerically model the viscoelasticity of blood, a patient-specific Womersley model as the inlet velocity profile and a patient-specific 3-element Windkessel model for the outlet pressures.

The results indicate that the developed computational tool is able to calculate the FFR, and its results display some high relative errors, of around 12%. In the case of Patient 1, that had a hemodynamic significant stenosis, the invasive FFR is 0.58, and the numerical FFR obtained through the tool is 0.50. For Patient 2, with a hemodynamic insignificant stenosis, the invasive FFR is 0.81 and the numerical FFR value is 0.90. It is known that an FFR lower than 0.75 means the stenosis is hemodynamically significant, and if the FFR is higher than 0.80, the stenosis is considered insignificant.

Therefore, even though the error of our tool is relatively high (>5%), the difference between the invasive and the computational FFR values seems to indicate that the tool can accurately categorize if the stenosis being studied is mild or severe.

In the future, many more patient-specific cases must be analyzed to validate the tool before it can be used on-site at the hospital by physicians to compute the FFR and aid in the diagnosis and treatment of coronary diseases.

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