Abstract

The geometry configuration of vascular bypass grafts has profound influence on the physiologic flow pattern. Poor geometries might be correlated with postoperative occlusion pathogenesis. Improving the blood flow dynamics in the bypass is an important element for the long-term success of bypass surgeries. Genetic algorithms are effective tools to identify optimal shapes of grafts given a robust fluid dynamics numerical solver able to determine the main flow features of different setups. This paper focuses on a specific graft shape and three design variables: graft calibre, graft angulation and suture sizing. A multi-objective shape optimization algorithm considers a genetic algorithm iterating over numerically simulated flow through idealized bypass grafts. Shape optimization is accomplished by simultaneously minimizing shear stress and recirculation zones.

Keywords: blood flow simulation, multi-objective optimization, genetic algorithms.

1 Introduction

Nowadays the ability to detect localized atherosclerotic plaques using non-invasive ultrasonic methods has advanced significantly. Atherosclerotic plaques tend to be localized at sites of branching and artery curvature, locations expected to harbour complex flow patterns. Currently, a working hypothesis for the role of fluid dynamics in postoperative pathogenesis is that intimal thickening is a normal response to low wall shear stress and that the spatial location of atherosclerotic plaque is related to the presence of oscillatory shear stress in those regions where transient flow reversal is prominent [1, 2]. Poor post-operative bypass graft performance is often attributed to the development of intimal hyperplasia (IH), a cell unnatural growth (restenosis) mechanism, at the graft distal junction. Research on the complexity of blood flow in the complete model of arterial bypass suggests that flow in the bypass graft is greatly dependent on the area reduction in the host artery.
As the area reduction increases, higher stress concentration and larger recirculation zones are formed at the distal corner of the bifurcation as well as at the toe and heel of the distal anastomosis that could be damaging to the artery-graft junctions. Searching an improvement of the blood dynamics conditions, shape optimization frameworks have been considered to optimize the geometry of artificial grafts [4 - 6].

The purpose of this research is to contribute towards the improvement of arterial bypass surgeries based on simulated models. Specifically, multi-objective shape optimization of an idealized artificial graft is presented. The process entails the combination of three computational entities: a finite element code solver, an automated pre-processor and a shape optimization genetic algorithm. The shape optimization will be accomplished by simultaneously minimizing shear stress and recirculation zones.

## 2 The finite element method formulation

The blood flow in the graft/artery system can be considered as incompressible and pulsatile by nature. The blood non-Newtonian rheology is accounted for through the Casson non-Newtonian model [7]. The hemodynamics problem is considered laminar since the anastomotic flow typically reaches a maximum Reynolds number less than 1000. The governing equations for this problem are the Navier–Stokes set that consists of the continuity and the momentum equations

\[
\begin{align*}
\rho \left( \frac{\partial u}{\partial t} \right) + \rho \left( u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) &= -\frac{\partial p}{\partial x} + \mu \nabla^2 u \\
\rho \left( \frac{\partial v}{\partial t} \right) + \rho \left( u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) &= -\frac{\partial p}{\partial y} + \mu \nabla^2 v \\
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0
\end{align*}
\]  

(1)

where \((u,v)\) is the velocity vector, \(p\) the pressure, \(\rho\) the density, \(\mu\) the dynamic viscosity and operator \(\nabla^2\) is defined as

\[
\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}
\]  

(2)

The dynamic viscosity varies spatially due to its dependence on the shear rate. The non-linear expression of \(\mu\) is given by the Casson law [7]

\[
\mu = \frac{\left( k_0 + k_1 \sqrt{2 \frac{\partial H}{\partial t}} \right)^2}{2 \sqrt{\frac{\partial H}{\partial t}}}
\]  

(3)

with \(k_0 = 0.6125, \ k_1 = 0.174\) and

\[
D_H = \frac{1}{2} \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right]
\]  

(4)
The arterial wall is assumed to be rigid. Regarding boundary conditions, a pulsatile waveform is prescribed at the inlet and a no-slip condition (zero velocity) is prescribed at the walls.

The developed numerical procedure [8] for the transient non-Newtonian equations uses the Galerkin-finite element method and a fractional-step method for the integration in time [9]. The discretization in time is obtained by an implicit fractional step-method in which the time advancement is decomposed into a sequence of two [9-11]. The method includes a diffusion term, which allows the imposition of full boundary conditions for the velocity while needing no pressure boundary conditions.

3 The graft geometry

Simplified arterial graft prosthesis is formed of a cylindrical tube disposed about the longitudinal axis of the prosthesis. The graft is symmetric and meets the host artery with a side-to-end proximal anastomosis and an end-to-side distal anastomosis. The host artery is assumed to be a fully stenosed straight conduit. As usually adopted by most previous investigations, the distensibility of the vessel wall is neglected. All the vessels are assumed to be impermeable rigid tubes. To our knowledge, most authors consider circular [12] or polynomial [4] symmetric geometries for the prosthesis with variable junction angles. Small junction angles have more obvious advantages for the hemodynamics of bypass grafts [12]. With a circular prosthesis, the optimal limit for junction angle would be close to zero producing an extremely large graft/artery junction. Instead of circular geometries, this investigation will consider sinusoidal geometries with the longitudinal axis of the graft being drawn by a sine curve. Figure 1 presents a simplified bypass model. There are at least three parameters that can be controlled: the suture line dimension, D, the width of the prosthesis, Wp, and the distance from the near wall of the graft to the near wall of the artery, H.

![Figure 1. Anastomotic configuration and nomenclature of the geometry model.](image)

The artery is simulated using a cylindrical tube of diameter 10 mm. For the shape optimization problem presented here, the graft is properly connected to the artery always in the same region. The space design of the three parameters is given as follows:
Only symmetric geometries were considered since removing the symmetry constrain does not have a significant effect [4].

4 The multi-objective GA

Genetic Algorithms (GAs), a family of biology-inspired methods, are considered here. With a GA a highly effective search of the solution space is performed, allowing a population of strings representing possible solutions to evolve through basic genetic operators. The goal of the genetic operators of the algorithm is to progressively reduce the space design driving the process into more promising regions. GA has many advantages, such as the capability of exploring a large design space, the merit that no gradients information is needed and also it can compute multiple independent objective functions simultaneously in one optimization run.

A general multi-objective optimization seeks to optimize the components of a vector-valued objective function mathematically formulated as

\[
\begin{align*}
\text{Minimize} \quad & F(b) = (f_1(b), \ldots, f_m(b)) \\
\text{subject to} & \quad b_i^{\text{lower}} \leq b_i \leq b_i^{\text{upper}}, \quad i = 1, \ldots, n \\
& \quad g_k(b) \leq 0, \quad k = 1, \ldots, p
\end{align*}
\]

where \(f_j(b)\) is the \(j\)th objective function, \(b = (b_1, \ldots, b_n)\) is the design variable vector, \(b_i^{\text{lower}}\) and \(b_i^{\text{upper}}\) represent the lower and upper boundary of the \(i\)th design variable \(b_i\), and \(g_k(b)\) the \(k\)th constraint.

Unlike single objective optimization approaches, the solution to this problem is not a single point, but a family of points known as the Pareto-optimal set. Typically, there are many Pareto optimal solutions for a multi-objective problem. Thus, it is often necessary to incorporate user preferences for various objectives in order to determine a single suitable solution. The weighted sum method for multi-objective optimization problems [13] continues to be used extensively not only to provide multiple solution points by varying the weights consistently, but also to provide a single solution point that reflects preferences presumably incorporated in the selection of a single set of weights. In this work, using the weighted sum method to solve the multi-objective optimization problem entails selecting random scalar weights \(w_j\) and minimizing the following composite objective function:

\[
\phi(b) = \sum_{j=1}^{m} w_j f_j(b)
\]
If all of the weights are positive, as assumed in this study, then minimizing Equation (8) provides a sufficient condition for Pareto optimality, which means that its minimum is always Pareto optimal.

For a shape optimization application, the GA process begins by randomly setting an initial population of possible individuals, where each individual represents a graft geometry. The successive populations maintain the same number of individuals as it evolves throughout successive generations. Each individual is referred to as a chromosome containing the binary representation of its design variables referred to as genes of the chromosome to which genetic operators are applied. Operators such as selection, crossover, mutation and elimination supported by an elitist strategy are considered to ensure that fitness of the forthcoming generations is always improved [14, 15]. The optimization scheme includes the following steps: Coding, the design variables expressed by real number are converted to binary number; Initialization, individuals of an initial population are produced randomly each representing a random geometry within the design variable space; Evaluation, fitness of each individual is evaluated using a defined optimization goal and individuals are ranked according to their multi-objective fitness value; Selection of the progenitors, one from the best-fitted group (elite) and another from the least fitted; Crossover, this operator builds a new chromosome by a multipoint combination technique applied to the binary string of two selected chromosomes; Mutation, the implemented mutation is characterized by changing a set of bits of the binary string corresponding to one variable of a randomly selected chromosome from the elite group; Elimination, deletion of the worst solutions with low fitness simulating the natural death of low fitted individuals. The original size population is recovered and a new population obtained; finally, Termination, checking the termination condition. If it is satisfied, the GA is terminated. Otherwise, the process returns to step Selection.

### 4.1 Shape optimization objective functions

Regarding the choice of suitable objective functions for the graft optimization problem, several different approaches have been pursued in the literature. The most frequently considered quantities in the context of blood flow are based on either shear stress or the flow rate. Unlike the situation at the suture line where injury and graft-artery compliance mismatch play a main role, the development of the IH on the host artery floor is thought to be purely caused by fluid mechanics factors. The two-dimensional wall shear stress (WSS) magnitude is expressed such as:

\[
WSS = \mu \| \mathbf{t} \| \tag{9}
\]

where \( \mathbf{t} \) is the traction vector with components:

\[
\mathbf{t} = \left( 2 \frac{\partial u}{\partial x} n_x + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) n_y , \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) n_x + 2 \frac{\partial v}{\partial y} n_y \right) \tag{10}
\]

where \( n_x \) and \( n_y \) are respectively the x- and y-components of the outward drawn unit normal vector at the boundary. High WSS gradient (WSSG) values are expected at
the floor occurring at the end-to-side distal area where there is flow recirculation and stagnation resulting from the flow impingement. The WSSG is essentially a tensor, and considering the tensor entries that tangentially affect the endothelial cells the two-dimensional objective function can be expressed as

$$ f_1(b) = \frac{1}{N_f} \sum_{i=1}^{N_f} \|WSSG\| $$

where $N_f$ is the number of boundary points on the floor optimization section.

The development of disease occurs preferentially in regions close to the proximal and distal anastomosis and their after effects are more critically correlated with the long-term effectiveness of bypass graft procedures [16]. For each simulation of an idealized bypass graft four domains of enhanced reversed flow and long residence time zones were identified: $\Omega^*_i, i = 1, \ldots, 4$, being $\Omega^*_1$ and $\Omega^*_2$ the reversed flow and the long residence time zones near the proximal junction and $\Omega^*_3$ and $\Omega^*_4$ the reversed flow and the long residence time zones near the distal junction, respectively. Reversed flows were assigned whenever negative longitudinal velocities are detected and long residence time zones when a significant area has associated mean velocities lower than 5 mm s$^{-1}$. Then minimizing long residence times corresponds to maximize the summation of the simulated longitudinal velocity $v_x$ at each elementary element of that critical domain,

$$ f_2(b) = -\sum_{\Omega^*_i(b)} v_x, i = 1, \ldots, 4 $$

Using scalar weights randomly generated, the following composite function

$$ \phi(b) = w_1 f_1(b) + w_2 f_2(b) $$

is considered for the optimization problem investigated in this work. The fitness function to be maximized by the GA is then defined as:

$$ FIT = A - \phi(b) - P $$

being $A$ is a positive integer to ensure positiveness and $P$ a value to penalize design vectors that do not conform with constraints as given in Eq. (5).

5 Shape optimization results and discussion

In this project the goal is to search the optimal shape of an artificial graft using a multi-objective genetic algorithm. The associated design vector considers three geometric parameters: the suture line dimension, D, the width of the prosthesis, Wp, and the distance from the near wall of the graft to the near wall of the artery, H.

Mesh of a simplified version of a sinusoidal bypass graft is shown in Figure 2 (flow direction going from left to right). The graft is symmetric and meets the host artery with a side-to-end proximal anastomosis and an end-to-side distal
anastomosis. Wall shear stress gradient is a critical hemodynamic parameter that should be considered, as high WSSG values indicate the presence of disturbed flow conditions such as separation and reattachment, stagnation point and re-circulation. These flow patterns occur at the end-to-side distal anastomosis IH prone sites. For the WSS and WSSG calculations involved in the optimization process, the location on the artery of the wall opposite to the end-to-side distal junction is presented in Figure 2.

![Figure 2. Mesh and end-to-side WSS location for the model](image)

As a compromise between computer time and population diversity, parameters for the genetic algorithm were taken as $N_{pop} = 12$ and $N_e = 5$ for the population and elite group size, respectively. The number of bits in binary codifying for each design variable is $N_{bit} = 5$ making a chromosome of 15 genes. This will correspond to a solution accuracy of 0.16 mm for variables $D$ and $Wp$ and 1 mm for variable $H$. The GA termination has been defined by fixing the total number of generations as 300. For each generation 6 new individuals (five from crossover plus one from mutation) are created, so 6 new blood flow numerical simulations are needed for every new generation. With a CPU time of 6 seconds for a typical finite element simulation is 6 seconds the total time for an optimization run is around 3 hours. One obtained optimal bypass geometries corresponds to parameters

$$
D = 12.7 \, mm \\
H = 19.8 \, mm \\
Wp = 11.65 \, mm
$$

(15)

Simulation results for the optimized bypass graft are presented in Figures 2 and 3.

![Figure 3. Velocity contours for the optimal graft model](image)
The velocity results are given in terms of longitudinal distribution. The velocity contours demonstrate the good quality of the finite element simulation being capable of capturing the flow acceleration as it emerges from the graft to the artery and the flow recirculation at the floor of the host artery, consistently with the expectations. It is interesting to notice that although the abrupt connection between artery and graft induces large velocity variations, the observable reverse flow is quite small. Long residence times usually observable immediately after the toe of the distal anastomosis are quite undetectable.

Regions of high WSS appear around stenosis at the distal corner of the proximal bifurcation and at the toe of the distal anastomosis. The computed WSS distribution at the floor of the host artery near the distal anastomosis for the optimal sinusoidal graft is shown in Figure 4.

![Figure 4. WSS at the artery floor for the optimized graft](image)

As expected, the WSS takes the highest values in the vicinity of the heel at the proximal junction. Around this region, very large WSS gradients are expected corresponding to the high blood impingement at the artery floor on the way out of the graft. The lowest shear stress regions are found on the arterial wall opposite to the junction, which are predominantly susceptible to the occurrence of artery plaque formation diseases.

Concluding, the present shape optimization is based on a GA and their objective functions are to reduce the WSSG on the floor of the host artery and the oscillatory flows expected at the artery graft junction area. The optimal value for H, distance from the near wall of the graft to the near wall of the artery, is too close to the constraint upper limit. This suggests that future numerical research should discuss the enlargement of the design space. It was found that not only the H distance is important but also that the caliber plays an important role in affecting the values of the WSS gradients on the host artery floor. Our results indicate that the graft caliber should be always maximized. The choice of optimal parameters comes as a trade-off between minimizing the WSSG and minimizing the spatial location of long residence times.
Peripheral arterial disease is estimated to affect millions individuals in the world. Arterial duplex imaging provides direct anatomic and physiologic information, but it does not provide information regarding the overall hemodynamics. Duplex imaging distinguishes between a stenosis and an occlusion, determines the length of the disease segment and patency of the distal vessels, evaluates the results of intervention (angioplasty, stent placement, bypasses), diagnoses aneurysms and pseudo-aneurysms of peripheral vessels such as the carotid arteries. From this study recommendations to vascular surgeons on how to consider their arterial anastomoses cannot be expected; however future recommendations will be potentially made once, among others, the blood transient nature is accounted for in the optimization process. The study reported herein establishes the methodology as a viable means of achieving optimal artificial graft shapes.

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