Multi-objective shape optimization of the human carotid artery

K. Vijaya Bhaskar,* Neil W. Bressloff, Prasanth B. Nair

Computational Engineering and Design Group, School of Engineering Sciences, University of Southampton, Highfield, Southampton SO17 1BJ, UK

Abstract

A statistical analysis is performed on the key geometric parameters that influence hemodynamics in the human carotid artery bifurcation. A parametric CAD model of the bifurcation is used to automatically construct a range of different geometries. A design of experiments (DoE) approach is employed to generate a set of candidate geometries for flow analysis using an unsteady three dimensional Navier–Stokes solver. The values of the integral of negative average shear stress (INASS) and the maximal average shear stress (MASS) corresponding to these geometries are then used to construct a Bayesian surrogate model. A shape optimization problem is proposed using the surrogate model which predicts arterial geometries having minimal INASS and MASS.

Keywords: Carotid artery; Bayesian modeling; Geometry; Optimization

1. Introduction

Due to the nature of the geometry and the hemodynamics in the human carotid artery, arterial disease commonly occurs in this region. Well-established correlations already exist between the geometric factors and the development of disease. An optimal arterial design strategy could be a useful tool for clinicians in search of a robust surgical procedure.

The present work draws on the techniques developed in Bhaskar et al. [1] for designing an optimum shape for the carotid artery via minimization of a suitable objective function using a Y-shaped parametric CAD model of the human carotid artery. A DoE technique is used to generate a set of candidate geometries at which the flow solver is run. The data generated from these simulations is then used to construct a Bayesian interpolant which approximates the desired objective function as a function of geometric variables. INMSS and MASS are considered as objective functions to be minimized in the shape optimization study. The paper concludes by discussing the application of Bayesian modeling to arterial graft/stent design.

* Corresponding author. E-mail: kvb@soton.ac.uk

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2. Overview

2.1. Bayesian modeling

A Bayesian approach is employed for surrogate modeling in order to efficiently optimize computationally expensive functions. Consider a deterministic computational fluid dynamics (CFD) code which takes as input the vector $\mathbf{x} \in \mathbb{R}^p$ and returns a scalar output $y(\mathbf{x})$. Further, for a given set of l input vectors $\mathbf{X} = \{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^l\} \in \mathbb{R}^{p \times l}$ the corresponding output values $\mathbf{y} = \{y^1, y^2, \ldots, y^l\} \in \mathbb{R}^l$ are assumed to be available. This training data can be obtained by applying a DoE technique to decide geometries at which the flow solver should be run. Using this *training data*, the approximation problem involves the prediction of the output $y(\mathbf{x})$ given a new design point $\mathbf{x}$.

The metamodel used in Bayesian interpolation can be compactly written as

$$Y(\mathbf{x}) = \beta + Z(\mathbf{x}) \tag{1}$$

where β is an unknown hyperparameter to be estimated from the data and $Z(\mathbf{x})$ is a Gaussian stochastic process with zero-mean and covariance

$$\mathrm{Cov}\big(Z(\mathbf{x}^1, \mathbf{x}^2)\big) = \sigma_z^2 R(\mathbf{x}^1, \mathbf{x}^2) \tag{2}$$

where $R(.,.)$ is a correlation function that can be tuned to the data and σ_z^2 is the process variance.

Assuming Gaussian prior over functions, and by applying Bayes' theorem, it can be shown that the posterior distribution is Gaussian [2], i.e. $Y(\mathbf{x})|\mathbf{y} \sim \mathcal{N}(\hat{Y}(\mathbf{x}), \sigma_z^2 C(\mathbf{x}, \mathbf{x}'))$. The posterior mean and covariance can be computed as

$$\hat{Y}(\mathbf{x}) = \beta + \mathbf{r}(\mathbf{x})^T \mathbf{R}^{-1}(\mathbf{y} - \mathbf{1}\hat{\beta}) \tag{3}$$

and

$$C(\mathbf{x}, \mathbf{x}') = \sigma_z^2 \Big(R(\mathbf{x}, \mathbf{x}') - \mathbf{r}(\mathbf{x})^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{x}') \Big) \tag{4}$$

where $\mathbf{R} \in \mathbb{R}^{l \times l}$ is the correlation matrix computed using the training points: the ijth element of this matrix is computed as $\mathbf{R}_{ij} = R(\mathbf{x}^i, \mathbf{x}^j)$. $\mathbf{r}(\mathbf{x}) = \{R(\mathbf{x}, \mathbf{x}^1)\, R(\mathbf{x}, \mathbf{x}^2) \ldots R(\mathbf{x}, \mathbf{x}^l)\} \in \mathbb{R}^l$ is the correlation between the new point $\mathbf{x}$ and the training points, and $\mathbf{1} = \{1, 1, \ldots, 1\} \in \mathbb{R}^l$.

It can be observed from Eqs. (3) and (4), that the Bayesian inferencing approach leads to an approximation of the CFD code as a multidimensional Gaussian random field. The posterior covariance given in equation (4) can be interpreted as an estimate of the uncertainty involved in making predictions at a new point $\mathbf{x}$.

2.2. Geometry model and methodology

It has already been observed that the bifurcation region is most vulnerable to arterial disease [3]. Further, the probability of plaque rupture, plaque ulceration and thromboembolism is maximum near the bifurcation region and more specifically on the inner walls of the internal carotid artery (ICA) [1]. In addition to this, studies have been performed to prove that the bifurcation angles affect the magnitude of reversed velocity and the extension of recirculation region near the sinus bulb [4,5]. Hence, with reference to Fig. 1, in the present study the widths proximal to the bifurcation – the upstream width of the ICA (Location 3; Mean – 8.3 mm), a width governing the shape of the sinus bulb (Location 4; Mean – 8.9 mm), the downstream width of the common carotid artery (CCA) (Location 5; Mean – 8.0 mm) – and the bifurcation angles (Location 1 with Mean – 25.1° and Location 2 with Mean – 25.4°) are used as input variables for creating the training data. Note that these are the key geometric variables which have been identified from previous studies [1,4]. To construct the surrogate model, 50 design points were created using the Latin-Hypercube sampling (LHS) technique [6]. The perturbation of each parameter in the design space is taken as 50% of the corresponding parameter's mean value. The geometries were created in CATIA V5 and the CAD files were exported in STEP format to GAMBIT for mesh generation. FLUENT was used for 3D unsteady simulations. The laminar incompressible momentum equations were solved and the viscosity was assumed to be constant at 0.0035 kg/m.s. The objective function values, INASS and MASS, were extracted for each geometry to create the training data for constructing the surrogate model.

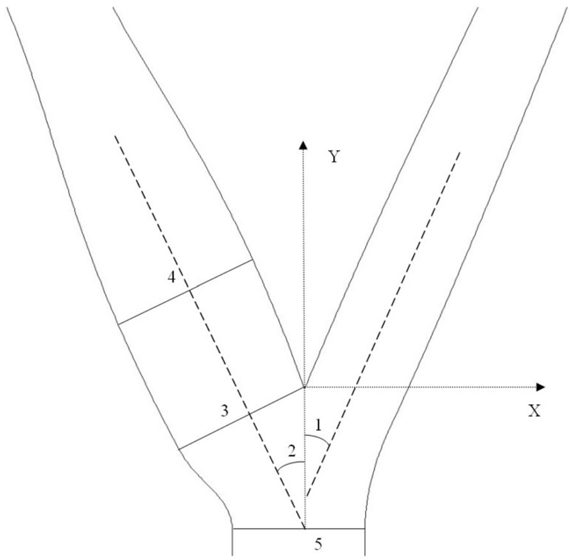

Fig. 1. Geometry of the human carotid artery.

3. Results and discussion

A mean pulse for the human carotid artery, as described in [7], was used with a time step of 0.0001 s. The meshes with a fixed interval size of 0.48 were employed on each geometry. These spatial resolutions were already used and validated in [1]. The density of blood was taken as 1035 kg/m^3. The mass flow split ratio between the ICA and the external carotid artery (ECA) was taken as 70 : 30. Due to the high perturbations assumed for the input variables to create the training data, 6 out of the 50 design points failed to create a valid arterial geometry. Hence, the surrogate model was created using the remaining design points.

The objective of the optimization study is to predict geometries which have low values of INMSS and MASS. The motivation for simultaneously minimizing INMSS and MASS arises from the fact that these metrics quantify different flow behaviors. The MASS is related to the elevated shear stress regions and the INASS is related to the negative shear regions and the amount of recirculation [8]. Hence, by taking these two metrics into account, the aggregate objective function will quantify the relationship between the geometry variations and the majority of the diseases occurring near the bifurcation. A good geometry with a minimal

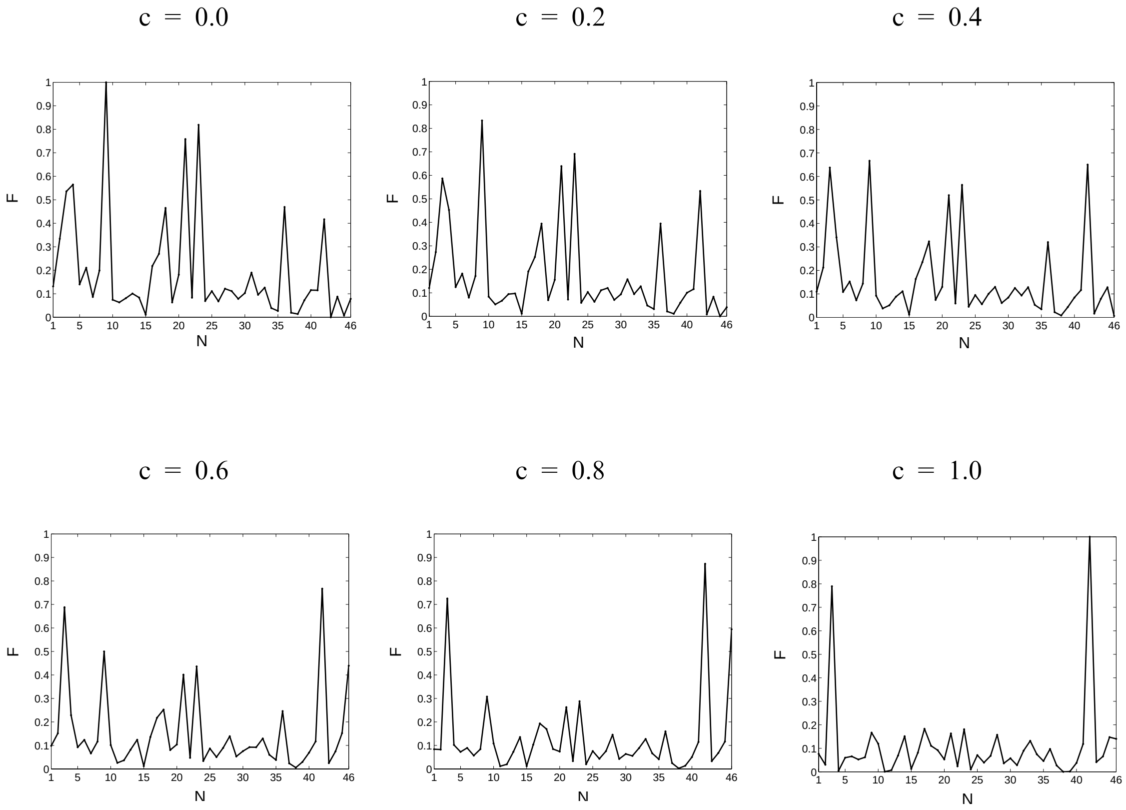

Fig. 2. Variation of the multi-objective function for different values of c. F denotes the normalized objective function and N denotes the number of geometries.

risk of disease is expected to have minimum values of INMSS and MASS. The underlying belief is that the resulting geometry will give rise to an optimum shape of the carotid artery.

The objective function chosen for the present study is of the form

$$F(\mathbf{x}) = cf_1(\mathbf{x}) + (1 - c)f_2(\mathbf{x}) \tag{5}$$

where $c \in [0,1]$ is a weighting factor and f_1, f_2 denote the two metrics INASS and MASS, respectively. After the simulations were performed for the 44 geometries, the values of INASS and MASS were extracted to construct $F(\mathbf{x})$ for values of $c = \{0, 0.2, 0.4, 0.6, 0.8, 1.0\}$. Further, surrogate models were constructed to approximate $F(\mathbf{x})$ for all the six values of c. This was achieved by employing the error bar predicted by the surrogate and maximizing the following probability of improvement (PoI) criterion.

$$\textbf{Maximize} : \mathrm{P}[Y(\mathbf{x}) < F^{-1}] \tag{6}$$

where F^{-} denotes the minimum value of $F(\mathbf{x})$ among all the geometries used as the training data. Note that the metrics INASS and MASS have been appropriately normalized before creating $F(\mathbf{x})$ using the maximum and minimum values of the metrics in the training data.

Using the above criterion these six cases are supposed to give rise to a set of non-dominated solutions due to the compromise obtained with each single objective function. However, by visual inspection of the data, it was found that the two metrics chosen were found not to conflict with each other. It was found that the geometry corresponding to a minimum INASS also had a low value of MASS.

The geometries obtained by maximizing the PoI criterion on the training data set will give rise to a better shape of the carotid artery compared to the initial configurations. Note that this criterion can also be used for updating the surrogate model to find a better optima. The new points obtained can be appended to the initial training data set and the criterion can be applied in an iterative fashion to find better geometries. This iterative

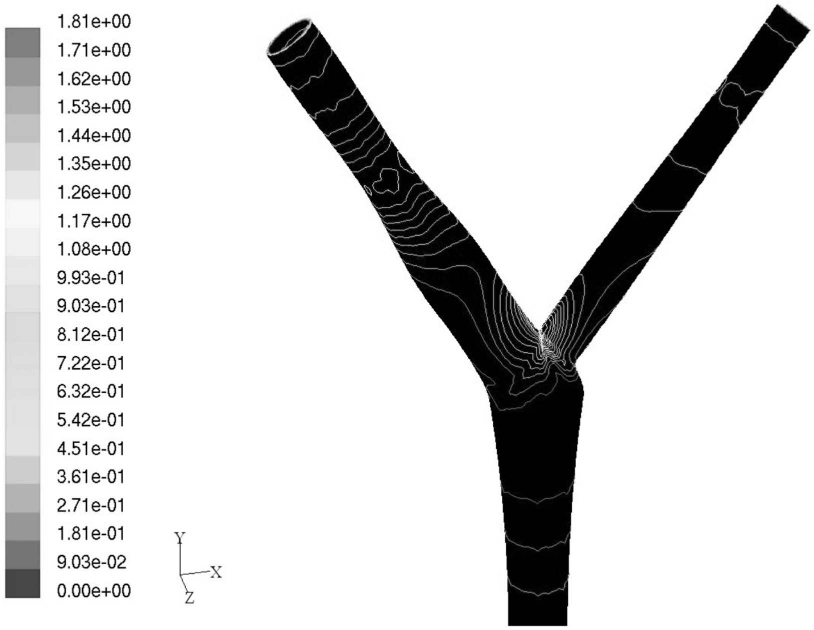

Fig. 3. Contours of wall shear stress (in *Pa*) of the optimal geometry (Time = 9.17e-01 sec).

procedure can be stopped by imposing some convergence criterion. This methodology works fine when the simulations carried to obtain the training data are cheap to run. Note that in the present case we are dealing with 3D pulsatile simulations which are very time consuming. Each numerical simulation takes about 14.5 CPU hours on an AMD Athlon XP 2800+ processor. Thus, the update procedure was conducted only twice. Figure 2 shows the variation of the objective function with the initial set of 44 geometries and the two geometries obtained after employing the update strategy for each value of c. The best geometry obtained after the update strategy is shown in Fig. 3. It can be seen in the Fig. 3 that the widths 3 and 4 were adjusted in such a way that the flow into the ICA promoted smaller reversed flow, thereby reducing the probability of plaque formation at the sinus bulb. The magnitudes of the downstream width of the CCA and the bifurcation angles for the best geometry were found to be greater than their corresponding mean values. The increase in the width 5 reduced the flow velocity entering the bifurcation region, which in turn influenced the shear stress distribution downstream.

4. Conclusions

An approach to determine the geometry that simultaneously minimizes the INASS and MASS in a 3D pulsatile flow of the human carotid artery is presented. Key geometric parameters near the bifurcation were varied to create several configurations. It was found that the individual INASS and MASS minimum configurations do generally coincide. The present study aims at highlighting the approach and giving a flavor of the results rather than exhaustively examining all of the possibilities. Ultimately, these optimal design capabilities can be used to handle patient specific geometric design of arterial grafts and stents.

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