INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
Int. J. Numer. Meth. Fluids 2005; **47**:1411–1419
Published online 21 January 2005 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/fld.888

On optimization, control and shape design of an arterial bypass[‡]

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SUMMARY

Multi-level geometrical approaches in the study of aorto-coronaric bypass anastomoses configurations are discussed. The theory of optimal control based on adjoint formulation is applied in order to optimize the shape of the incoming branch of the bypass (the toe) into the coronary. At this level, two possible options are available in shape design: one implements local boundary variations in computational domain, the other, based on the theory of small perturbations, makes use of a linearized design in a reference domain. At a coarser level, reduced basis methodologies based on parametrized partial differential equations are developed to provide (a) a sensitivity analysis for geometrical quantities of interest in bypass configurations and (b) rapid and reliable prediction of integral functional outputs. The aim is (i) to provide design indications for arterial surgery in the perspective of future development for prosthetic bypasses, (ii) to develop multi-level numerical methods for optimization and shape design by optimal control, and (iii) to provide an input–output relationship led by models with lower complexity and computational costs. We have numerically investigated a reduced model based on Stokes equations and a vorticity cost functional (to be minimized) in the down-field zone of bypass: a Taylor like patch has been found. A feedback procedure with Navier–Stokes fluid model is proposed based on the analysis of wall shear stress-related indexes. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: optimal control; shape design; small perturbations; flow control; parametrized PDEs; generalized Stokes problem; reduced basis methods; arterial bypass optimization

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‡Bill Morton CFD Prize paper, ICFD 2004, Oxford, U.K.

Contract/grant sponsor: EU-RTN, European Union Research Training Network, HaeMOdel Project; contract/grant number: HPRN-CT-2002-00260

Received 27 April 2004
Revised 15 September 2004
Accepted 18 October 2004

1. FRAMEWORK: CFD IN HAEMODYNAMICS

When a coronary artery is affected by a stenosis, the heart muscle cannot be properly oxygenated through blood. Aorto-coronaric anastomosis restores the oxygen amount through a bypass surgery downstream an occlusion. At present, different kinds and shapes of aorto-coronaric bypass anastomoses are available and, consequently, different surgery procedures are used to set up a bypass. A bypass can be made up either by organic material (e.g. the saphena vein taken from patient's legs or the mammary artery) or by prosthetic material. Prosthetic bypasses are less invasive. They may feature very different shapes for bypass anastomoses, such as, e.g. cuffed arteriovenous access grafts.

Mathematical modelling and numerical simulation of physiological flows allow a better understanding of phenomena involved in coronary diseases (see References [1, 2]). Improvement in the understanding of the genesis of coronary diseases is very important as it allows the reduction of surgical and post-surgical failures. It may also suggest new means in bypass surgical procedures as well as with less invasive methods to devise new shapes in bypass configuration (see Reference [3] for an introduction to optimal design for arterial bypass anastomosis).

1.1. A geometrical multi-level investigation

The background provided by mathematical modelling and numerical simulation has led us to apply the optimal control theory of systems governed by partial differential equations (PDEs) with the aim of optimizing the (full) configuration and the (local) shape of a simplified bypass model. In support to this aim at macro-geometrical level efficient schemes for reduced-basis methodology [4] applied to parametrized partial differential equations (P^2DEs) are being used to provide useful and quick indications (outputs) in a repetitive design environment as shape design requires. With the reduced basis approach also a sensitivity analysis of the initial configuration and a study of important geometrical quantities in bypass can be obtained (see Reference [5] for an introduction and Reference [6] for details). Figure 1 clarifies our geometrical double-level of interest for bypass design.

1.2. Two control approaches

At micro-geometrical level, optimal control of one (or several) aspects of the problem entails the minimization of a *cost functional* which describes physical quantities involved in the

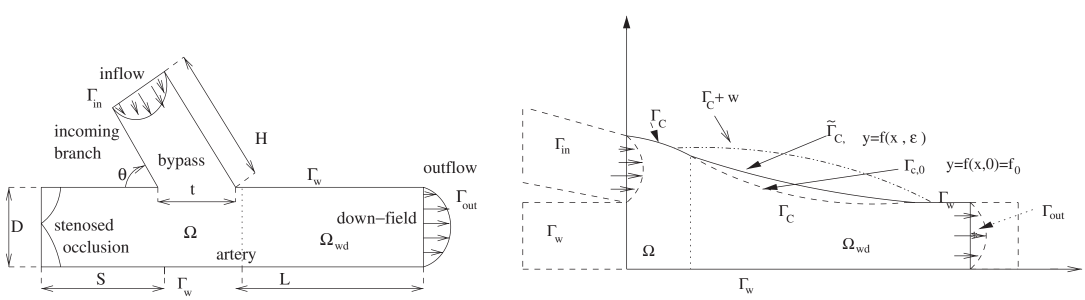

Figure 1. Bypass schemes: macro geometrical (left) and local configurations (right).

specific problem. The problem is related both to *optimal shape design* (see Reference [7]) and *flow control* (involved in the observation of the evolving system and in cost functionals (such as vorticity or wall shear stress)). The optimization process is carried out by a *control function* used as parameter in modelling the shape of the domain. At this level, two control approaches have been used: in the former, the control function is used to define directly the boundary shape (local boundary variation method) in the true domain (see Reference [8]); in the latter, the control function is used to define the mapping transformation from the reference domain to the true one. In this case, the design problem becomes an optimal control problem on coefficients and the analysis is based on small perturbation theory (see Reference [9]). In both cases, the adjoint approach proposed by Lions [10] to get cost functionals gradient in a problem with distributed or boundary control and observation has been developed. In the functional optimization process, a descent gradient-type method (with fixed optimized step size) is used. Numerical approximation is based on the Galerkin-finite element method, with Taylor–Hood elements P^2 and P^1 for velocity and pressure, respectively, see Reference [11].

1.3. Results and feedback

At the end of a first investigation stage, preliminarily reported in Reference [8], based on optimal design by local boundary variation, a cuffed bypass is found with a shape which resembles the Taylor arterial patch [12]. Results reported in Section 4, based on the multi-level control approaches, go in the same direction, using a different initial configuration. The effect of the shape obtained is to reduce gradually the average velocity of the blood as it approaches the distal anastomosis, since the cross-sectional area of the bypass is steadily becoming larger. This prevents the sudden deceleration experienced in the conventional model with the fluid returning to the host vessel. Blood flows more smoothly through the vessel thanks to the gradually changing geometry. Consequently, there is a smooth reduction of the momentum of the blood while approaching the junction. Flow disturbances are abated and undesirable flow separation at the toe of the bypass diminished. Vorticity reduction by the optimization process is quite substantial. A feedback procedure has then been implemented by solving the unsteady Navier–Stokes equations in the original configuration as well as in the final configuration obtained after applying the shape optimization process on the simplified model. The quadratic functional used at this stage to take into consideration wall shear stress variations in time t (T is the heart beat) and along the vascular wall Γ_w (Figure 1) reads

$$J_\tau = \text{mean}_{0\leqslant t\leqslant T}\ \Sigma(t) = \frac{1}{T}\int_0^T \Sigma(t)\,\mathrm{d}t = \frac{1}{T}\int_0^T\int_{\Gamma_w}\left(\frac{\partial}{\partial t}\tau_w(t)\right)^2 \mathrm{d}\Gamma\,\mathrm{d}t \tag{1}$$

and it is the L^2 norm of the rate of the wall shear stress $\tau_w(t)$ defined (for a Newtonian fluid) as

$$\tau_w(t) = \mu\frac{\partial\mathbf{u}(t)}{\partial\hat{n}}\cdot\hat{\tau} \tag{2}$$

where $\mathbf{u}$ is the blood velocity field, μ the blood viscosity, $\hat{n}$ and $\hat{\tau}$ are respectively normal and tangential unit vector on the arterial wall. A reduction of 25% in wall shear stress spatial and temporal oscillations has been achieved.

1.4. Development guidelines

Optimal control and shape optimization applied to fully unsteady incompressible Navier–Stokes equations and the setting of the problem in a three-dimensional geometry will provide more realistic design indications concerning surgical prosthesis realizations. Theoretical investigation based on perturbation theory analysis and linearized shape design is providing results on the existence and uniqueness of the solution and about well-posedness of the problem, and is permitting us to better understand the problem from a theoretical point of view. Reduced-basis methodology approximation is going to provide not only high computational savings but also a methodological pre-process to detect the essential feature of the optimization process itself (such as a sensitivity analysis). The ultimate goal is to build an input–output relationship

$$s_i = F_i(\mu_k)$$

with different models characterized by an increasing degree of complexity, where s_i are outputs of interest (design quantities and fluid mechanics indexes) and μ_k are inputs (typically geometrical quantities).

2. CONTROL AND SHAPE DESIGN: A DOUBLE APPROACH

The Stokes equations in a two-dimensional computational domain Ω with velocity vector $\mathbf{u} = \{u, v\}$ and pressure p read

$$\begin{cases} -\nu\Delta\mathbf{u} + \nabla p = 0 \quad \text{in} \quad \Omega \subset \mathbb{R}^2 \\ \nabla\cdot\mathbf{u} = 0 \quad \text{in} \quad \Omega \\ \mathbf{u} = 0 \quad \text{on } \Gamma_{\mathrm{w}}, \quad \mathbf{u} = g_{\mathrm{in}} \quad \text{on } \Gamma_{\mathrm{in}}, \quad T\cdot\hat{n} = 0 \quad \text{on } \Gamma_{\mathrm{out}} \end{cases} \tag{3}$$

where $\hat{n}$ is normal unit vector on the boundary $\partial\Omega$. The latter is partitioned in three components: Γ_{in} is the inflow boundary, where a Hagen–Poiseuille's velocity profile g_{in} is imposed, Γ_{out} is the arterial outflow boundary, with a free-stress Neumann-type condition on stress tensor T, and Γ_{w} is the boundary corresponding to the arterial wall, the stenosed artery portion and the incoming branch of bypass with no-slip conditions imposed; Figure 1 represents schematically the computational geometry and the symbols used.

Velocity values at the inflow are chosen so that the Reynolds number has order 10^3. Blood kinematic viscosity ν is $4 \times 10^{-6}\,\mathrm{m}^2\,\mathrm{s}^{-1}$ [1].

In this first approach, the control w represents the shape of Γ_c: a part of Γ_{w} (typically the upper part of the incoming branch), made up of M branches $\Gamma_c^j(w) = \overline{\Gamma_c^j} + w^j$, where w^j is the control variable, the curves $\overline{\Gamma_c^j}$ represent initial shape. The control shape function w^j changes of a quantity δw^j during the optimization process (gradient-based method with optimized stepsize). At the kth iteration we have

$$w_k^j = \sum_{m=0}^{k-1} (\delta w_m^j) \tag{4}$$

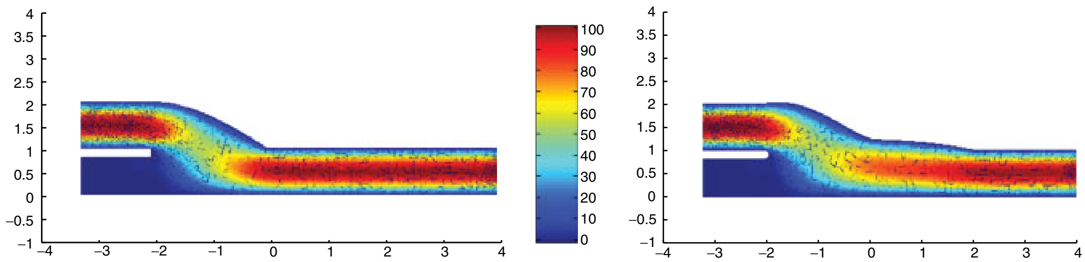

Figure 2. Bypass configuration (velocity [ms^{-1} 10^{-2}]) near the incoming branch before (left) and after shape optimization (right) by boundary variations (30 iterations, 40% vorticity reduction).

2.1. *The observation on the system*

We consider vorticity as distributed observation (flow control combined with shape optimization) in the down-field zone Ω_{wd} of the incoming branch of the bypass, defined as $\nabla \times \mathbf{u} = \partial v/\partial x - \partial u/\partial y$ and we control the system by minimizing the functional

$$J(w) = \int_{\Omega_{\mathrm{wd}}} |\nabla \times \mathbf{u}|^2 \, \mathrm{d}\Omega + \alpha \|w\|^2, \quad (\alpha \ll 1) \tag{5}$$

where the last term provides the minimum shape deformation and guarantees existence of the solution. During the optimization iterative process we must solve the following adjoint problem:

$$\begin{cases} -v\Delta \mathbf{q} + \nabla \pi = \nabla \times \nabla \times \mathbf{u}|_{\Omega_{\mathrm{wd}}} & \text{in } \Omega \\ \nabla \cdot \mathbf{q} = 0 \quad \text{in } \Omega, \quad \mathbf{q} = 0 & \text{on } \partial\Omega \end{cases} \tag{6}$$

where $\mathbf{q}$ and π denote the adjoint velocity and pressure, respectively. Adjoint problem solution represents sensitivity of the cost functional with respect to observation (state solution) and allows computational savings when computing $J'(w)$. In fact, $J'(w) = G(\mathbf{q}, \pi, w)$. At each iteration, we get a new shape variation by a gradient-based method (optimized λ stepsize $0 < \lambda \ll 1$)

$$\delta w_k^j = -\lambda J_k'(w_k^j) \tag{7}$$

In 30 iterations, we have a vorticity reduction of 40% (Figure 2). This approach needs a remeshing procedure to control the minimum angle and maximum side length of triangles facing the boundary during mesh stretching at each iteration. For more details see [8].

2.2. *Small perturbations*

A second approach to local shape design is based on a map from the real domain Ω to a (rectangular) reference one $\tilde{\Omega}$ using a variable transformation

$$\tilde{x} = x, \quad \tilde{y} = \frac{1}{f(x,\varepsilon)} y \tag{8}$$

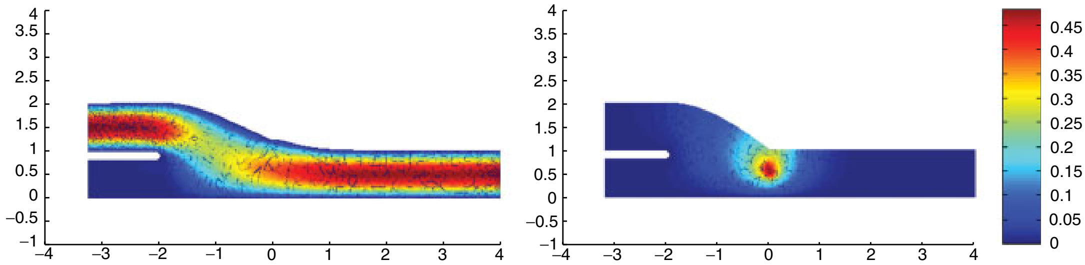

Figure 3. Bypass configuration (velocity [$\mathrm{ms}^{-1}\,10^{-2}$], same colourbar of Figure 2, 25 iterations and 30% vorticity reduction) after design by small perturbations (left) and its adjoint solution in reference domain (right). Adjoint solution underlines the most sensible zone related with observation.

where $f(x,\varepsilon)$ represents the upper shape and can be developed as

$$f(x,\varepsilon) = f_0(x) + \varepsilon f_1(x) + \varepsilon^2 f_2(x) + \cdots \tag{9}$$

$f_0(x)$ being the unperturbed shape. Assuming that problem (3) has a solution $\mathbf{u}, p$ that is infinitely differentiable with respect to ε

$$\mathbf{u} = \mathbf{u}_0 + \varepsilon \mathbf{u}_1 + \varepsilon^2 \mathbf{u}_2 + \cdots$$

$$p = p_0 + \varepsilon p_1 + +\varepsilon^2 p_2 + \cdots$$

and using small perturbation techniques (see Reference [13]), we can derive the equations for $\mathbf{u}_k, p_k$ starting from (3), after mapping Ω to the reference domain. At this point, we can use optimal control techniques to solve the problem for $\mathbf{u}_1, p_1$ (the first corrections), the function $f_1(x)$ represents a perturbation in the shape $f_0(x)$ (weighted by ε) and is another unknown for the problem, used as control variable. As in the first approach, we use an adjoint formulation, a gradient-type method and the same functional (observation). In this case, the shape design problem is transformed into an optimal control problem on the coefficients, which depend on the co-ordinate transformation itself. Results are shown in Figure 3 in 25 iterations we achieve a vorticity reduction of about 30%, while a theoretical analysis is reported in Reference [9]. Masmoudi *et al.* [14] have investigated a complementary approach based on high-order derivatives and Taylor expansion of the cost functional with respect to shape parameters.

3. REDUCED BASIS TECHNIQUES FOR PRE-PROCESS

Reduced basis techniques (see, e.g. References [4, 15]) are used here for a pre-process applied to macro bypass configuration (Figure 1), more precisely in order to obtain quantitative information about sensitivity of some geometrical quantities before applying local shape design.

Table I. Table of velocity H^1 and pressure L^2 relative errors, $N \leqslant 20$.

N	Rel. err. H^1 max	Rel. err. H^1 mean	Rel. err. L^2 max	Rel. err. L^2 mean
5	$2.93e-001$	$7.86e-002$	$3.09e-002$	$6.14e-003$
10	$1.33e-002$	$4.47e-003$	$6.79e-003$	$6.96e-004$
15	$2.98e-003$	$6.65e-004$	$8.16e-004$	$9.02e-005$
20	$4.61e-004$	$8.01e-005$	$6.24e-004$	$1.60e-005$

By selecting a limited number of relevant geometrical parameters (bypass diameter t, artery diameter D, stenosis length S, graft angle θ, bypass bridge height H, see Figure 1) and a number (N) of sample parameters

$$\mu_k = \{t_k, D_k, S_k, \theta_k, H_k\}, \quad k = 1, \ldots, N$$

we solve the state Equations (3) in a reference domain $\tilde{\Omega}$, properly mapped by affine transformations [5]. Then we build a (reduced) basis functional space

$$\zeta = \{\mathbf{u}_k(\mu_k), \sigma_k(\mu_k)\}, \quad \xi = \{p_k(\mu_k)\}, k = 1, \ldots, N$$

for velocity and pressure, respectively. Note that ζ has been enriched by additional velocity $\sigma_k(\mu_k)$, which are the so-called Supremizer solutions. These extra functions allow the spaces ζ and ξ to satisfy a compatibility condition similar to the inf–sup condition [11]. The supremizers are the weak solutions of the problem

$$-\Delta\sigma_k + \sigma_k = \nabla p_k \tag{10}$$

For a new sample μ we look for a solution

$$\mathbf{u}_N = \sum_{k=1}^{2N} U_k(\mu)\zeta_k(\mu_k), \quad p_N = \sum_{k=1}^{N} P_k(\mu)\xi_k(\mu_k)$$

where the weights $\mathbf{U} = \{U_k\}$ and $\mathbf{P} = \{P_k\}$ are given by the solution of a Stokes problem on the subspace of the reduced basis (see Reference [6] for details).

This approach can provide an indication on the flow pattern perturbation. Increasing, for example, the bypass graft angle from $\theta_k \cong 0$ to $\pi/2$, the mean blood velocity increases about 43% (testing hundreds of different configurations μ_k with a subspace built on $N = 20$ basis functions). Table I shows max and mean relative errors (H^1 for velocity and L^2 for pressure) over the same test samples.

4. SOME NUMERICAL RESULTS

We present below some numerical results obtained by applying both the optimal control by local boundary variation (Figure 2) and the small perturbations techniques (Figure 3), starting from the same configuration with a small graft angle and a cuffed upper part (as suggested

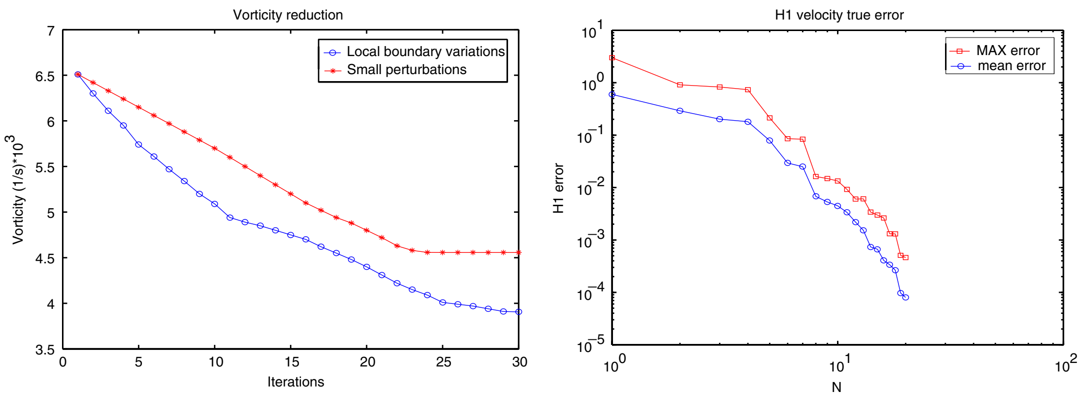

Figure 4. Vorticity reduction achieved during the two optimization processes: shape design by local boundary variations and small perturbations (right). Relative H^1 velocity error (max and mean) testing a large number of bypass configurations using reduced basis and increasing N (left).

by results in Reference [8]). The Shape is smoothed at the intersection with the artery to guide blood, and the corner (singularity) disappears. Figure 4 shows the reduction of the cost functional (5) during optimization processes and H^1 error reduction (max and mean) during reduced basis pre-process at different N.

ACKNOWLEDGEMENTS

This work is being developed within the European Community's Human Potential Programme, HaeMOdel Project 'Mathematical Modelling in Haemodynamics'(contract HPRN-CT-2002-00260) and the Bernoulli Center of EPFL during the special semester on the 'Mathematical Modelling of the Cardiovascular System'. I acknowledge Prof. A. Quarteroni (MOX-Politecnico di Milano and EPFL) for guidelines dealing with haemodynamics and mathematical modelling, C. Prud'homme (EPFL), Prof. A. T. Patera and K. Veroy (MIT) for reduced basis tools applied to PDEs, Prof. V. Agoshkov (Russian Academy of Sciences) for optimal control framework and adjoint problems in shape design.

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