VI International Conference on Computational Bioengineering
ICCB 2015
M. Cerrolaza and S.Oller (Eds)

COMPUTATION OF SENSITIVITY DERIVATIVES FOR PEDIATRIC VENTRICULAR ASSIST DEVICE USING THE ADJOINT METHOD

JOAO S. B. LIMA[1†], JOAO A. ISLER[1], ERNANI V. VOLPE[1], X. MAO[2], BRUNO S.CARMO[1] and IDAGENE A. CESTARI[3]

[1]University of São Paulo, Polytechnic - Mechanical Engineering Department
05508-970, Brazil

[3]University of São Paulo - Heart Institute. InCor – Medical School
05403-900, Brazil
[†]E-mail: joaobrasil.lima@usp.br

[2] Durham University, School of Engineering and Computing Sciences,
UK, DH1 3LE

Key words: Adjoint method, Optimization, Sensitivity analysis, Pediatric ventricular assist device, Fluid dynamics

Abstract. This work focuses on the application of the adjoint method to pediatric ventricular assist device (PVAD), in order to develop an optimization methodology capable of improving its performance. Equally important is the capability to compute sensitivity derivatives of relevant measures of merit with respect to operational parameters. On following the usual practice in the literature, we asume that the flow is governed by the Navier-Stokes equations. This particular study has the goal of obtaining the correspondent adjoint equations for this problem, as well as the appropriate set of boundary conditions. For this initial purpose a 2D computational mesh is used, the flow is assumed to be steady and an uniform velocity profile in imposed on the inlet of the PVAD. A set of relevant measures of merits is identified for the sensitivity analysis. The validation of flow and adjoint simulations, as well as of the gradient computations is discussed. This calculation is performed by using the adjoint-based gradient formula that will be shown in this paper. Preliminary results show that it is possible to make use of the adjoint method to compute sensitivity gradients pertaining to this class of devices. The validation of the methodology for gradient evaluation is the starting point of the optimization process of the PVAD.

1 INTRODUCTION

There is a rapidly growing literature on the use of Computational Fluid Dynamics (CFD) resources to investigate the blood-flow through the so-called Ventricular Assist Devices (VAD). Of particular interest to us, a recent study [1] points out the importance of CFD in the design process of those devices. With the appropriate experimental validation [3], CFD resources should enable one to accurately predict flow behaviour inside different configurations of VADs, thus opening up the possibility of optimizing them.

However, it is well-known that those flows are highly complex, owing to the rheology of blood and its non-Newtonian character. Moreover, the flow behaviour, itself, may lead to complications of biological nature, such as haemolysis, thrombosis and emboli, which must be avoided. Even more so when it comes to pediatric patients, in view of the smaller displacement volumes and higher pumping frequencies of the paediatric devices (PVAD), which increase the incidence of the aforementioned complications [2]. Although many of these issues have not been sufficiently resolved in the literature, in principle, they should be taken into account in the design and optimization of PVADs.

The adjoint method is a powerful tool to tackle these issues, in that it enables one to capture the flow physics with high fidelity in the optimization process. It also allows for a systematic exploration of the space of realizable solutions, at a cost that is virtually independent of the number of design parameters. In particular, our approach to the method [4] provides a means for one to evaluate the sensitivity of flow measures to parameters other than those concerning the device geometry. In principle It extends the method capabilities to flow parameters such as Reynolds number, inflow velocity profiles and pulsation frequency.

This work focuses on the application of the adjoint method to PVADs, where the blood is modelled as a Newtonian incompressible fluid. Hence the flow is governed by the usual Navier-Stokes equations. The continuous form of the adjoint equations are presented, along with the appropriate boundary conditions [4]. A set of relevant measures of merit is identified, and their sensitivity gradients are evaluated and discussed. Numerical simulations shall be carried out by making use of high order codes [5],[6]. In order to validate the methodology for the calculation of the sensitivity gradients, the simulations will be performed in a 2D computational mesh, with no moving boundaries and with an uniform velocity profile on the inlet of the device. The most important steps of the derivation of the adjoint equations and the sensitivity gradient formula are presented what follows.

2 THE ADJOINT METHOD

2.1 General Formulation of the Adjoint Method

In general, measures of merit that are relevant to fluid-dynamics applications, involve functionals or functions of the flow variables, U and its geometry $\mathcal{F}$ [7,8]:

$$I = I(U, \mathcal{F}) \tag{1}$$

Usually, $\mathcal{F}$ is represented as a function of the flow coordinates and a set of parameters α. Geometry variations $\delta\mathcal{F}$ can occur as a result of parameter variations ($\delta\alpha$), which then cause variations in the flow variables δU. In that regard, it is possible to obtain an expression for the sensitivity gradient of the measure of merit I with respect to geometry parameters α:

$$\frac{\partial I}{\partial \alpha}=\frac{\partial I}{\partial U}^T\frac{\partial U}{\partial \alpha}+\frac{\partial I}{\partial \mathcal{F}}^T\frac{\partial \mathcal{F}}{\partial \alpha} \tag{2}$$

By considering all four terms that are required for the gradient calculation, the second one, $\partial U/\partial \alpha$ is hardly ever known in closed form – that is, except for a very few cases of little practical interest. This derivative could be calculated by using finite differences, but the computational cost becomes prohibitive whenever the number of parameters α increases. For example, if $\mathcal{F}$ contains N parameters, at least N+1 numerical simulations will be necessary to compute the derivative – one for the baseline solution plus one for each of the parameters which must be perturbed separately.

The general principle of the adjoint method is to restrict the physical variations to a locus of realizability by imposing the flow governing equations as constraints on the variational problem. It assumes that the solution to those equations depends on the flow variables and on its boundaries geometry:

$$R(U,\mathcal{F})=0 \tag{3}$$

Therefore, all the realizable variations δU must satisfy the condition $\delta R=0$, i.e.:

$$\delta R=\frac{\partial R}{\partial U}\delta U+\frac{\partial R}{\partial \mathcal{F}}\delta \mathcal{F} \tag{4}$$

The restriction is introduced in the variational problem by multiplying it by a Lagrange multiplier ψ and by adding it to the variation of the measure of merit δI:

$$\begin{gathered}\delta I=\frac{\partial I}{\partial U}^T\delta U+\frac{\partial I}{\partial \mathcal{F}}^T\delta \mathcal{F}-\psi^T\left(\frac{\partial R}{\partial U}\delta U+\frac{\partial R}{\partial \mathcal{F}}\delta \mathcal{F}\right)\\ \delta I=\left[\frac{\partial I}{\partial U}^T-\psi^T\frac{\partial R}{\partial U}\right]\delta U+\left[\frac{\partial I}{\partial \mathcal{F}}^T-\psi^T\frac{\partial R}{\partial \mathcal{F}}\right]\delta \mathcal{F}\end{gathered} \tag{5}$$

The Lagrange multiplier ψ is chosen so as to satisfy the eq. (6),

$$\frac{\partial R}{\partial U}\psi=\frac{\partial I}{\partial U} \tag{6}$$

Which eliminates the first term in equation (5), and the variation of the measure of merit becomes independent from the flow variations δU. The surviving terms give rise to the following expression for δI

$$\delta I=\left[\frac{\partial I}{\partial \mathcal{F}}^T-\psi^T\frac{\partial R}{\partial \mathcal{F}}\right]\delta \mathcal{F} \tag{7}$$

The independence of eq. (7) from δU allows one to compute the sensitivity gradient with respect to any number of parameters, without the need for any additional flow simulation [9,10,11].

2.2 The Adjoint Problem for Incompressible Navier-Stokes Flows

In the applications that are considered here, the main objective is to find flow configurations that represent extrema of a given measure of merit. That measure is usually a functional of the flow variables. That is, an integral over the body surface $\mathcal{B}$. For the PVAD problem there are some measures of merit that are relevant, such as the fluid stress tensor, vorticity and forces. In this work, as a preliminary test, the measure of merit chosen is the force exerted by the fluid (blood) on the PVAD walls, projected onto a given direction $\boldsymbol{e}$:

$$I_0 = \frac{1}{T}\int_0^T \oint_B G(\boldsymbol{n}.\boldsymbol{\sigma}.\boldsymbol{e})dS\, dt \tag{9}$$

where $\sigma = \tau - pI$ represents the fluid stress tensor. The well-known Navier-Stokes equations are given by:

$$\begin{cases} \partial_0\boldsymbol{u} + (\boldsymbol{u}.\nabla)\boldsymbol{u} + \nu\nabla p - \nu\nabla^2\boldsymbol{u} = 0 \\ \nabla.\boldsymbol{u} = 0 \end{cases} \tag{10}$$

Hence, the augmented functional can be written as:

$$I = \int_0^T \oint_B G(\boldsymbol{n}.\boldsymbol{\sigma}.\boldsymbol{e})\left|\frac{dS'}{dS}\right| dS\, dt + \frac{1}{T}\left\{\int_\Omega \theta\nabla\boldsymbol{u}\, d\Omega - \int_\Omega \psi[\partial_0\boldsymbol{u} + (\boldsymbol{u}.\nabla)\boldsymbol{u} + \nu\nabla p - \nu\nabla^2\boldsymbol{u}]d\Omega\right\} \tag{11}$$

It is possible to calculate the first variation of the augmented functional, and then, to separate physical variations from those pertaining to control parameters. Then, by means of Gauss's Theorem one can transfer to the adjoint variables the differential operators that are originally applied to the physical ones. To a large extent, the procedure relies on the fundamental hypothesis that all physical variables are continuous and differentiable within the domain. Fortunately, it is reasonable to expect such behavior of the pressure and velocity fields, under the flow conditions that are considered here. The final expression obtained is

$$\begin{aligned} T\delta I = & \int_\Omega \{\varphi^{\mathrm{j}}\big|_j \nu\delta p + [\partial_0\varphi_{\mathrm{i}} - u^j\varphi_{\mathrm{i}}|_j + \varphi_{\mathrm{j}}u^j|_i + \Theta|_i - \nu(\varphi_{\mathrm{i}}|^j + \varphi^{\mathrm{j}}\big|_i)|_j\,]\delta u^i\}d\bar{\xi}dt + \\ & - \int_0^T \oint_{\partial\mathcal{D}} \left\{[u^j\varphi_{\mathrm{i}}n_j - \Theta n_i + \nu\left(\varphi_{\mathrm{i}}|_j + \varphi_{\mathrm{j}}\big|_i\right)n^j]\delta u^i + \nu(\delta p n^i - \delta\mathcal{F})\varphi_{\mathrm{i}}\right\}dS\, dt + \\ & - \left[\int_{\mathcal{D}} \varphi_{\mathrm{i}}\delta u^i dV\right]_0^T + \int_0^T \oint_B \left[\frac{\partial G}{\partial p}\delta p + \frac{\partial G}{\partial \mathcal{F}^k}\delta\mathcal{F}^k\right]\left|\frac{dS'}{dS}\right| dSdt + \\ & + \int_0^T \oint_B G\delta\left|\frac{dS'}{dS}\right| dS\, dt + \int_\Omega \frac{\Theta}{J}\left[\delta\left(J\beta^k_{q'}\right)u^{q'}\right]_{,k} d\Omega \\ & - \int_\Omega \frac{\varphi_{r'}}{J}\left\{\partial_0\left(\delta J u^{r'}\right) + \left[\delta\left(J\beta^j_{n'}\right)\left(u^{r'}u^{n'} + g^{r'n'}p\nu - \nu u^{r'}_{,p'}g^{p'n'}\right)\right]_{,j}\right\}d\Omega \end{aligned} \tag{12}$$

The first four integrals concern only physical variations, while the last two involve only geometry variations. In essence, the rationale behind the method is to derive the adjoint equation and boundary conditions so as to drive the integrals containing physical variations, to zero. The first domain integral, gives rise to the adjoint equations, as a means of driving it to zero for arbitrary physical variations δu and δp.

$$\begin{cases} \partial_0\varphi_{\mathrm{i}} - u^j\varphi_{\mathrm{i}}|_j + \varphi_{\mathrm{j}}u^j|_i + \Theta|_i - \nu\varphi_{\mathrm{i}}|^j|_j = 0 \\ \varphi^{\mathrm{i}}|_i = 0 \end{cases} \tag{13}$$

where φ is the adjoint velocity vector and Θ is the adjoint pressure. The adjoint boundary conditions are obtained by pursuing the same rationale with the second and fourth integrals of eq. (12). The third integral corresponds to the time conditions and it is driven to zero by assuming that $\varphi|_{t=T} = 0$. The set of adjoint boundary conditions is given below:

Table 1: Set of boundary conditions for viscous incompressible flows. Flow and adjoint BCs

Contour	**Flow**	**Adjoint**
Inflow	$u^i = f(\xi^j, t, \alpha^k)$	$\boldsymbol{\varphi} = 0$
Outflow	$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{n}} = 0$ $p\ fixed$	$\frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{n}} = -\frac{(\boldsymbol{u}.\boldsymbol{n})\boldsymbol{\varphi}}{\nu}$ $\Theta = 0$
Wall	$\boldsymbol{u} = 0$	$\boldsymbol{\varphi} = -\rho \frac{\partial \mathrm{G}}{\partial \mathcal{F}} \left\vert \frac{dS'}{dS} \right\vert$
Symmetry Plane	$\boldsymbol{u}.\boldsymbol{n} = 0$ $\frac{\partial \boldsymbol{u}^t}{\partial \boldsymbol{n}} = \frac{\partial p}{\partial \boldsymbol{n}} = 0$	$\boldsymbol{\varphi}.\boldsymbol{n} = 0$ $\frac{\partial \boldsymbol{\varphi}^t}{\partial \boldsymbol{n}} = \frac{\partial \Theta}{\partial \boldsymbol{n}} = 0$

The remaining terms in eq. (12) represent the sensitivity gradient.

$$T\delta I = \int_0^T \oint_B G\delta \left|\frac{dS'}{dS}\right| dS\, dt + \int_\Omega \frac{\Theta}{J}\left[\delta\left(J\beta^k_{q'}\right)u^{q'}\right]_{,k} d\Omega + \\ - \int_\Omega \frac{\varphi_{r'}}{J}\left\{\partial_0\left(\delta J u^{r'}\right) + \left[\delta\left(J\beta^j_{n'}\right)\left(u^{r'}u^{n'} + g^{r'n'}p\nu - \nu u^{r'}_{,p'}g^{p'n}\right.\right.\right. \tag{14}$$

As for control parameters that are not related to the flow geometry, they are also imposed as variational constraints on the problem. In essence, they control the inflow boundary conditions and thus, they are not subject to the integrations by parts, performed by means of Gauss's Theorem. For the sake of space, we refer the reader to references [4,12] for further details on this portion of the derivation. The final expression for the sensitivity gradient reads:

$$< a, \delta\alpha >= \int_0^T \oint_{S_i} [\nu(\varphi_i|_j + \varphi_j|_i)n^j - \Theta n_i] \frac{\partial f^i}{\partial \alpha^k} \delta\alpha^k dS\, dt \tag{15}$$

where S_i is the inflow boundary and α is a (or more) non-geometrical parameter.

3 PRELIMINARY RESULTS

3.1 Parameters of the PVAD

Below, a PVAD is shown as means of illustrate the assembly of this device:

Figure 1: Photo of PVAD

The PVAD considered in this work is the one shown below:

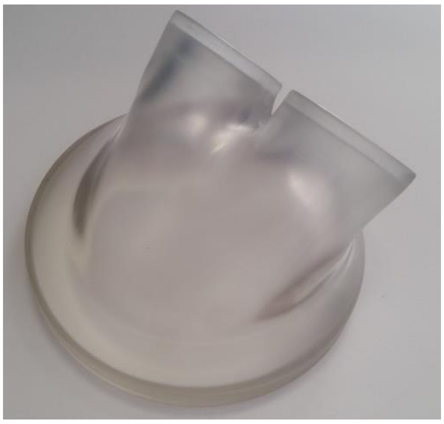

Figure 2: Photo of the PVAD considered in this work

The mesh for numerical simulations will be extracted from the 3D geometry of a PVAD characterized by the following parameters:

Table 2: Parameters of the PVAD

Parameter	**Value**
Inlet diameter	$22\ mm$
Outlet diameter	$14\ mm$
Volume	$35\ mL$
Inclination with horizontal	$35\ °$
Angle between cannulas	$8\ °$

The 2D mesh was obtained from a slice of the 3D geometry, as shown below:

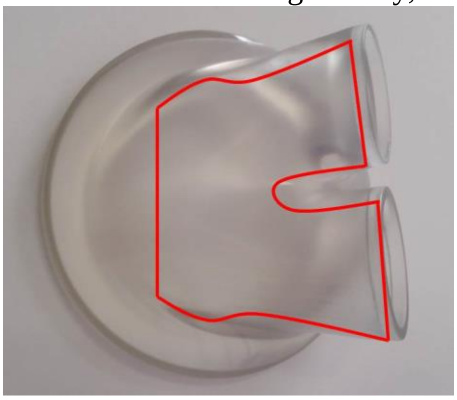

Figure 3: In red, the slice from the 3D geometry that was used to generate the 2D mesh

3.2 Geometry of PVAD and Simulation Mesh

The 3D geometry that was used to extract the 2D geometry in order to generate he simulation mesh is:

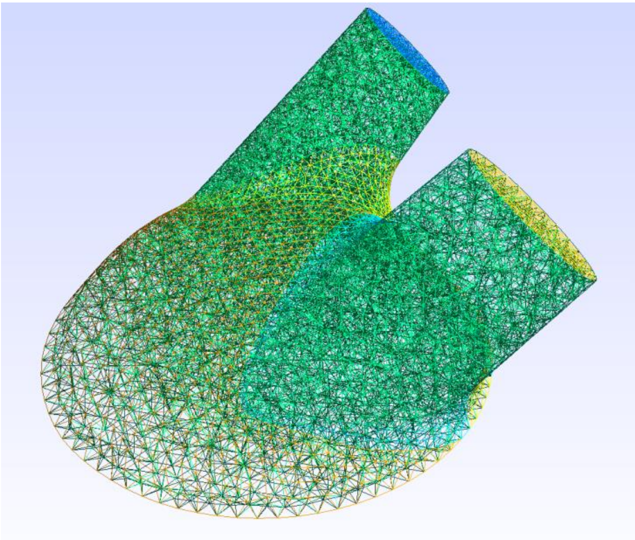

Figure 4: 3D geometry of the PVAD

The 2D was generated in the software Gambit (ANSYS™) and it is shown below:

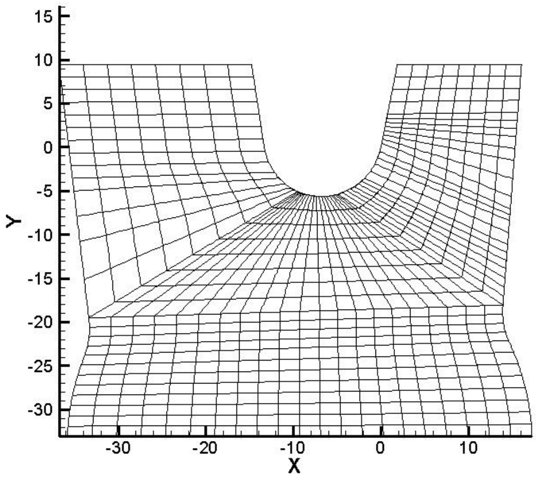

Figure 5: 2D mesh. Axes scales in mm

3.3 Results

The simulations were carried out in a high order numerical code [13] that is based on the spectral/hp element method. The inflow velocity adopted is $0{,}22\ m/s$, the viscosity of the blood as $\nu = 3{,}87.10^{-6} m^2/s^2$. That leads to a Reynolds number of $Re = 1249$, approximately. The simulation mesh contains 716 elements, the polynomial order is 10, the numerical time step is $dt = 0{,}0002$ and the number of time steps is 120000. The result of the flow simulation with these parameters is the following:

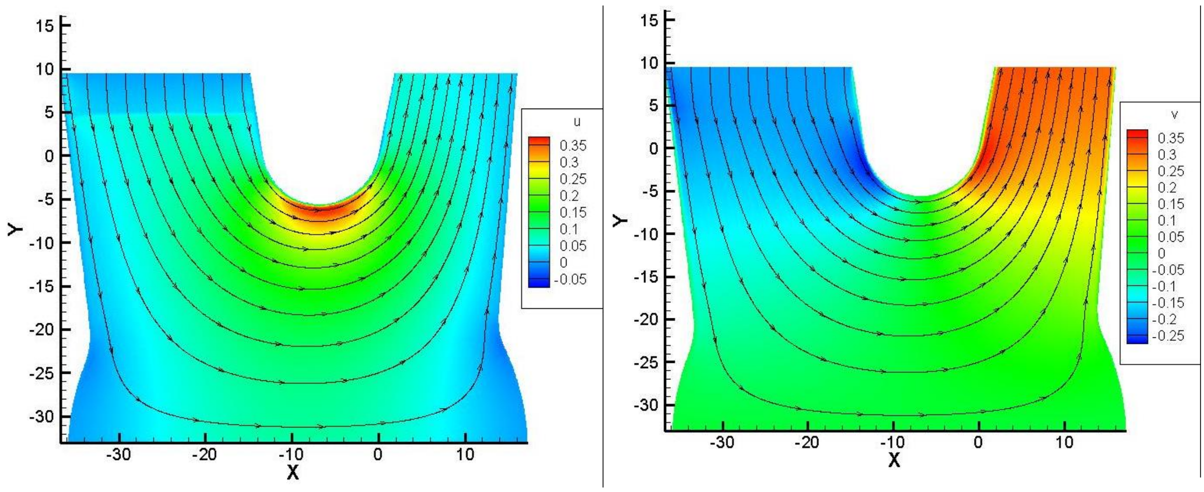

Figure 6: Flow solution. On the left, background colour-scale represents contours of horizontal velocity u, with particle path-lines. On the left, background colour-scale represents contours of vertical velocity v, also with particle path-lines.

The solution of the adjoint equations is the following:

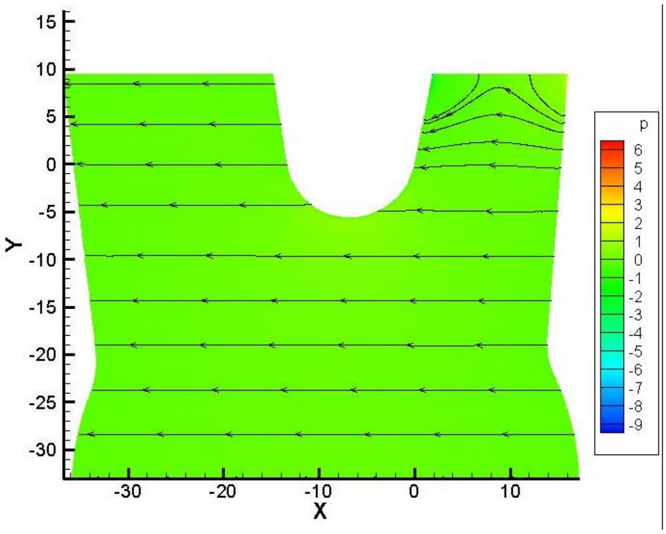

Figure 7: Adjoint solution, background colour-scale represents contours of adjoint pressure Θ

3.4 Computation of the Sensitivity Derivative

As a preliminary test to calculate the sensitivity of a measure of merit in respect to a control parameter, on calculate the sensitivity of the force that the fluid exerts on the PVAD projected in the x direction in respect to inflow velocity, using eq.(15), assuming steady flow:

$$\frac{\partial F_x}{\partial U_\infty} = \frac{1}{Re} \oint_S \{[\nabla\varphi + (\nabla\varphi)^{\mathrm{T}}] - \Theta\mathbb{I}\}\boldsymbol{n}\, dS \tag{16}$$

The integration is performed in the inflow boundary and the result is compared to the value of the same sensitivity derivative computed by finite differences. The preliminary results are:

Adjoint Method	Finite Differences
-0.0016	-0.0013

4 CONCLUSIONS

The preliminary results presented above, show that it is possible to make use of the adjoint method to compute sensitivity derivatives pertaining to this class of devices. Although more tests are still necessary to validate the process The main purpose of this work is to open the possibility of using the adjoint method to calculate the sensitivity derivatives to, in the future, compute derivatives that are more relevant to the analysis of the operation of the PVAD and to optimize it. Furher tests consists in compute the sensitivity derivatives in respect with Reynolds number, then change the inlet velocity profile to a pulsatile one, compute sensitivity derivatives in respect to the frequency of this profile, and, run new tests to other measures of merit.

ACKNOWLEDGEMENTS

This work is part of the Research Project "Circulatory Support in Paediatric Patients: Ventricular Assist Device and Extra-corporeal Membrane Oxygenation". It is a joint effort by researchers at the Heart Institute (InCor) of the Medical School and the Polytechnic of the University of São Paulo, who work under grant number FAPESP 2012/50283-6. The authors would like to acknowledge the financial support of FAPESP (São Paulo State Foundation for the Support of Research) that is provided for this project. J.S.B.L would like to acknowledge CAPES (Coordination for the Improvement of Higher Level -or Education- Personnel) for the scholarship that was provided during the development of this work.

REFERENCES

[1] K. H. Fraser, M. E. Taskin, B. P. Griffith, and Z. J. Wu. The use of computational fluid dynamics in the development of ventricular assist devices. *Medical Engineering and Physics*, 33:263-280, 2011

[2] E. Ferrara, M. Muramatsu, K. T. Christensen, and I. A. Cestari. Particle Image Velocimetry Study of a Pediatric Ventricular Assist Device. *Journal of Biomechanical Engineering*. 132, 2010

[3] B. N. Roszelle, S. Deutsch, and K. B. Manning. Flow Visualization of Three-Dimensionality Inside the 12cc Penn State Pulsatile Pediatric Ventricular Assist Device. *Annuals of Biomedical Engineering*, 38:439-455, 2010

[4] E. V. Volpe. Continuous Formulation of the Adjoint Problem for Unsteady Incompressible Navier-Stokes Flows. Technical Report 4, ANP NDF EPUSP, SP, June 2011. Research Project: ANP-CFD-ANFLEX, Desenvolvimento de Modelos Preditivos para Análise do Comportamento Dinâmico de Risers

[5] X. Mao. *Vortex Instability and Transient Growth*; PhD thesis, Imperial College of Science, Technology and Medicine, London, UK, 2010

[6] B. S. Carmo. On wake interference in the flow around two circular cylinders: direct stability analysis and flow-induced vibrations. PhD thesis, Imperial College, London, 2009

[7] A. Jameson and S. Kim. Reduction of the adjoint gradient formula for aerodynamic shape optimization problems. *AIAA Journal*, v. 41, n. 11, p. 2114-2129, November 2003.

[8] J.J. Reuthers. *Aerodynamic Shape Optimization Using Control Theory*; PhD thesis, University of California, 1996.r.

[9] O. Pirronneau. On optimal profiles in stokes flow. *Journal of Fluid Mechanics*, v. 59, n. 1, p. 117-128, 1973.

[10] A. Jameson. Aerodynamic design via control theory. In: *12th IMACS World Congress on Scientific Computation*. Paris: [s.n.], 1988. (MAE Report 1824).

[11] A. Jameson. *Optimum Aerodynamic Design via Boundary Control*. [S.l.], April 1994.

[12] D. G. Cacuci, C. F. Weber, E. M. Oblow and J. H. Marabale. Sensitivity theory for general systems of non-linear equations. *Nuclear Science and Engineering*, v. 75, p. 88110, 1980.

[13] D. Barkley, H. M. Blackburn and S. J. Sherwin. Direct optimal growth for timesteppers. *International Journal for Numerical Methods in Fluids*, v. 1, n. 231, p. 1-21, September 2002.